Shock-Induced Martensitic Phase Transitions II: Graphite, Diamond, and Iron
Oscar Bruno and Dimitri Vaynblat
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Dimitri Vaynblat and Oscar Bruno
Applied Mathematics MC 217-50, Caltech, Pasadena, CA 91125

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Abstract

In a companion paper we developed a theory for phase transitions in solids under shock-loading. There we showed that the single assumption that stresses in a phase cannot lie beyond the transition boundaries leads to a complete mathematical description of the physical problem at hand. In detail, our model only requires knowledge of well studied material observables: the equations of state (EOS) for the pure phases and the phase transition boundaries. We also presented a general Riemann solver for materials satisfying our main modeling assumption. In the present paper we utilize the previous work to construct general solutions for the piecewise constant initial value problems usually arising in experiment. Further, we specialize our solutions to two widely-studied polymorphic phase changes: the graphite-diamond transition and the $\alpha$--$\epsilon$ transition in iron. Our solutions are in close agreement with experimental results. Interestingly, in some cases our model predicts sequences of events which differ from those generally accepted.

1 Introduction

In the companion paper (Bruno & Vaynblat, 2000) we developed a theory for phase transitions in solids under shock-loading. In that article, which will be referred to as Part I in what follows, we showed that the single assumption that stresses in a phase cannot lie beyond the transition boundaries leads to a complete mathematical description of the physical problem at hand. In detail, our model only requires knowledge of well studied material observables: the equations of state (EOS) for the pure phases and the phase transition boundaries. In particular we showed that this theory gives rise to certain characteristic two-wave patterns associated with phase transitions under shock loading. In the present paper we use the Riemann solver introduced in Part I to solve a variety of initial value problems — which arise from application of our theory to a class of experimental setups commonly used. In particular we
produce explicit profiles for two widely-studied shock-induced polymorphic phase changes: the graphite–diamond transition (Erskine & Nellis, 1992) and the \( \alpha \rightarrow \epsilon \) transition in iron (Barker & Hollenbach, 1974). As shown in Section 4, our solutions are in close quantitative agreement with reported observables, and, interestingly, in some cases our theory predicts sequences of events which differ from those generally accepted — including the occurrence of Regimes B.1 and B.3 in Section 3.1 — compare (Barker & Hollenbach, 1974; Boettger & Wallace, 1997) — and the existence of a transformation front in in the second Riemann problem for Regime B of Section 3.2 — compare (Erskine & Nellis, 1992; Vlodarchik & Trebinski, 1997).

In the experiments under consideration phase transitions result from the impact of a planar projectile on the free surface of a flat slab. The impact occurs at the surface labeled ITI (Impactor-Target Interface); manifestations of the ensuing phenomena are recorded through the particle-velocity histories at the “Monitored Interface” (MI), that is, the surface opposite to the ITI. Such velocity histories are usually obtained by means of a VISAR interferometer. Typical experimental particle-velocity histories are shown in the left portions of Figure 5; these curves are manifestations of the wave structures induced within the target as a result of the impact.

The Riemann solver developed in Part I can be utilized to solve an arbitrary initial value problem — provided use is made of an appropriate shock-capturing numerical scheme. As we show below, however, many situations encountered in practice can be dealt through direct use of the Riemann solver and lead to essentially analytical approximate expressions for the solution. In essence, this can be accomplished if all wave interactions can be accurately approximated by interaction between discontinuities; see Section 2: in such approximations, rarefaction fans are substituted by rarefaction discontinuities.

Our notations are the same as in Part I; we use the notation (I-n) to refer to equation (n) of Part I. This paper is organized as follows: In Section 2 we construct closed-form approximate solutions for a certain class of initial value problems arising from our theory. In Section 3 we apply our theory to the experimental setups of (Barker & Hollenbach, 1974) and (Erskine & Nellis, 1992) and we describe all the possible evolution scenarios predicted by our theory in those contexts. Finally, in Section 4 we compare our predictions for phase transitions in iron and graphite with the corresponding results of experiment; a detailed discussion of the material parameters of the associated EOSs and critical curves is also included in this section.

2 Initial Value Problem

In this section we utilize the Riemann solver developed in Part I to construct closed-form approximate solutions for a certain class of initial value problems (IVP) arising from our theory. The importance of our approximate solutions is clear: they provide guidance in the construction of numerical schemes and, in fact, they apply and give correct quantitative results for some of the experimental configurations used most frequently. While our constructions do not contain explicit error estimates, comparisons with numerical results (Weatherwax et al., 2000) show
that the approximations we utilize here are very accurate indeed. All of the explicit comparisons with experiment presented in Section 4 are based on the approximate solutions given here.

Rarefaction waves constitute the main obstruction for explicit solution of an arbitrary one-dimensional IVP. Indeed, while interactions between one-dimensional discontinuities (shocks, transformation fronts and contacts) only require solution of Riemann problems (RP), interactions between discontinuities and rarefaction waves do require full numerical solution. Fortunately, in many configurations arising in practice, the rarefaction waves are sufficiently weak (Zel’ dovich & Raizer, 1967), so that they can be approximated accurately by rarefaction discontinuities.

2.1 Rarefaction Discontinuity Approximation

An assumption of weak waves — where the wave strength is measured by any of the three quantities \( [q]/q^a \) or \( [v]/v^a \) or \( [u]/v^aC^a \) — allows us to treat rarefaction fans as rarefaction discontinuities. As it happens, under such approximations all wave interactions can be resolved in closed form by the Riemann solver introduced in Part I. A validation of this approximation, further to be referred to as rarefaction discontinuity approximation, can be found in (Courant & Friedrichs, 1948). In particular, it follows from (Courant & Friedrichs, 1948, p. 156) that the expansive front curve (I-27)-(I-28) centered at a given ahead state \( \Sigma^a \) provides an approximation for the corresponding fan curve (I-32)-(I-33) with errors of the third order in the wave strength.

The solution of a Riemann problem obtained from a Riemann solver in which fan curves are replaced by the corresponding front curves contains only discontinuities and no fans. To quantify the errors introduced in the solution by this approximation we utilize the parameter \( \delta = [q]/q^a \) as a measure of the wave strength; as we mentioned the associated errors in the fan curve are of order \( O(\delta^3) \). Clearly, each one of the four constant states which make up the solution is approximated with an error of \( O(\delta^3) \); the speed of propagation of each discontinuity, in turn, being a quotient of jumps (each on of which is a quantity of order \( O(\delta) \)), is approximated with an error of \( O(\delta^2) \). It should be noticed that the replacement of a fan by the corresponding rarefaction discontinuity introduces a first order error in the approximate solution in the region of the \( (x, t) \)-plane which in the exact solution is covered by the fan. This region has itself a width of \( O(\delta) \). Indeed, the speed at which the fan spreads is given by the difference \( C^b - C^a \) of the Lagrangian velocities of the sound waves ahead of and behind the fan, and this difference is of the order of the wave strength. Thus, for time intervals below a certain bound — which depends on the particular problem at hand — the approximation is accurate.

Remark 1 Approximations of the type we utilize here have long been known in the solid dynamics community. A special case of this approximation — the “free surface approximation” — has been used widely in studies of rarefaction fans arising from reflection of shocks at free surfaces (Zel’dovich & Raizer, 1967). A detailed treatment of the degree to which the free surface approximation is valid can be found in (Walsh & Christian, 1955). The first explicit use of the “general” rarefaction discontinuity approximation in a Riemann solver can be attributed to (Colella, 1982). A detailed discussion of a Riemann solver in which fans are approximated
by discontinuities can be found in (Dukowicz, 1985).

2.2 Closed Form Solutions

In a typical experiment the impact induces one or two discontinuity fronts in the target and one or two discontinuity fronts in the flyer, c.f. Section 2 of Part I. These simple wave patterns account for the first stages of the experiment, up to the time when the leading wave reaches a material boundary — such as the free surface and the graphite-LiF interface in the experiments of (Barker & Hollenbach, 1974) and (Erskine & Nellis, 1992) respectively. For later times, however, the wave structure inside the impactor-flyer system is more complicated. It includes waves reflected from material boundaries, secondary waves born in interaction of reflected and incoming waves, etc, so that, as time evolves, many waves are generated through reflections and interactions.

All such reflections and interactions have been taken into account in the calculations leading to the predictions presented in this paper. Notwithstanding the large number of waves involved, the procedure to be followed in determining the complete solution to the impact problem is rather simple. This simplicity stems from the rarefaction discontinuity approximation introduced in the previous section, for which all waves are necessarily discontinuities. Since the impact-time data for target-flyer configurations is piece-wise constant, under our approximations all of the waves arising from such initial data must move with constant velocities and the state between any two waves must be a constant state.

In detail, the piece-wise constant data at the impact time \( t = t_1 \) gives rise to a RP which will be denoted by \( RP_1 \). This RP is centered at \( \xi_1 \), and its left and right states are the initial states of the flyer and the target, respectively. Thus, within the impactor and target the solution of the IVP resulting from the impact coincides with the solution of \( RP_1 \) up to a certain time \( t_2 \) at which a leading front reaches a material surface. For definiteness we assume the right facing leading wave is the first one to reach a material boundary — whose position we denote by \( \xi = \xi_2 \). Since, again, the data on the flyer-target system at time \( t_2 \) is piece-wise constant, the solution of the IVP can be continued by incorporating the solution of a new RP — which will be denoted by \( RP_2 \). This RP is centered at \( \xi_2 \) with left state equal to the constant state behind the front and right state equal to the state on the right side of the material surface. The solution of the impact problem for \( t > t_2 \), for \( t \) sufficiently close to \( t_2 \), is then constructed by piecing together the solutions to \( RP_1 \) and to \( RP_2 \). We thus note that, under the rarefaction discontinuity approximation, the solution continues to be piecewise constant for all times, and can thus be obtained by piecing together the solutions of a sequence of RPs — each one of which arises as discontinuities reach material surfaces or collide with each other.

In summary: under the rarefaction discontinuity approximation the complete solution to the impact problem is constructed by piecing together the solutions of the sequence of Riemann problems \( RP_1, RP_2, \ldots \). Each one of the waves that make up the solution is a discontinuity traveling at a constant speed. Each such discontinuity \( W \) is uniquely determined by three constants: its velocity \( s \) and the pair \( (\xi, t_i) \) giving the location of the RP at which this wave
was initiated. Further, the state $\Sigma$ lying between any two waves is uniquely characterized by a triple of constants $(v, q, u)$. Thus, the complete solution to the impact problem is determined if all pairs $(\xi_k, t_k)$ at which the fronts collide with each other or with material surfaces, all wave speeds $s$, and all the state triples $(v, q, u)$ are known.

3 Qualitative Predictions and Attainable Scenarios

A variety of possible scenarios may arise as a result of a flyer-target impact problem in a given flyer-target system. For example, relative strengths of waves may cause an interaction between a rarefaction discontinuity and a transformation front to produce either an advancing or a retreating transformation front. In this section we apply our theory to the experimental setups of (Barker & Hollenbach, 1974) and (Erskine & Nellis, 1992), and we describe all the possible evolution scenarios predicted by our theory — within the reported experimental time frames. To do this we construct the corresponding complete flows through consideration of a sequence of Riemann problems, as indicated in the previous section. These qualitative predictions are illustrated with figures which resulted from numerical simulations utilizing actual materials constants — which were obtained as indicated in Section 4. Corresponding quantitative comparisons of theory and experiment are also given in Section 4.

Unlike the discussion in Part I and in the previous sections, our presentation below utilizes the intuitively appealing Eulerian coordinates $(x, t)$.

3.1 $\alpha-\epsilon$ phase transition in iron

Sixteen out of the twenty experiments reported in (Barker & Hollenbach, 1974) used an experimental configuration containing iron-made targets and flyers without any added devices, so that the MI is a free surface. (The additional four experiments utilize either a sapphire impactor or a sapphire window in contact with the MI.) The velocity of the MI was measured as a function of time using a VISAR interferometer; see our depiction of these results in Figure 4, left. Experiments were carried out with various thickness of impactor and target and various impact velocities $u_f$.

In what follows we describe the possible evolution scenarios within the flyer-target system for the sixteen free-surface experiments mentioned above. We thus begin by considering the initial configuration $\Sigma(x, t_1)$ of states at the impact time $t = t_1$, for which we use the following notation:

$$
\Sigma(x, t_1) = \begin{cases} 
\Sigma_0^i, & x < x_1 \\
\Sigma_0^T, & x_1 < x < x_1 + L \\
\Sigma^V, & x_1 + L < x,
\end{cases}
$$

(1)
where $x_1$ is the (Eulerian) position of the ITI at impact time, $L$ is the initial length of the target, $\Sigma^I_0 = (v^I_0, 0, u^I_f)$ and $\Sigma^T_0 = (v^T_0, 0, 0)$ are the initial states in the impactor and target (which are in the austenitic phase, at zero stress, with specific volume $v^0$ as measured at room temperature, and moving with speeds $u^I_f$ and 0, respectively), and $\Sigma^V$ is the vacuum state, with $\rho^V = 0$, $q^V = 0$, and $u^V$ undefined. The data (1) defines the first RP: $RP_1$. According to this data, $RP_1$ is centered at $(x_1, t_1)$ with left state $\Sigma^L_1 = \Sigma^I_0$ and right state $\Sigma^R_1 = \Sigma^T_0$; the other RP arising from this data, which is centered at $(x_1 + L, t_1)$, has a trivial solution. (We point out that the experimental reference under consideration (Barker & Hollenbach, 1974) does not provide specifics concerning impactor size; our calculations, in turn, assume semi-infinite impactors. Finite impactors give rise to additional release waves originated from reflections of shocks from the back surface of the plate. Fortunately, however, these additional waves would lead to only negligibly small corrections to the computed observables in the time-ranges under consideration, see Section 4.1.)

Depending on the magnitude of the impact velocity $u_f$, the Riemann problem $RP_1$ will admit solutions of different types and, thus, it will give rise to different flow regimes. Three qualitatively different flow regimes shall be distinguished, corresponding to the three ranges of values of $u_f$ introduced in Section 2 of Part I.

**Regime A:** $u_f \leq u_f^{\text{crit}}$. A typical $(x, t)$-diagram is depicted in Figure 1 (a); the particular data used to construct this graph corresponds to experiment number 14 in (Barker & Hollenbach, 1974). In this regime only one discontinuity develops in the target upon impact, and only one discontinuity develops in the flyer. The solution to $RP_1$ (which is marked 1 in Figure 1 (a)) consists of four austenitic states $\Sigma^I_0$, $\Sigma^L_1$, $\Sigma^R_1$, and $\Sigma^T_0$ separated by three waves: a 1-shock front $W^I_1$, a contact discontinuity $W^C_1$, and a 3-shock front $W^R_1$. The contact discontinuity $W^C_1$ is the ITI, the interface between the impactor and the target. We note that $W^C_1$ is a degenerate contact discontinuity, that is, the states $\Sigma^L_1$ and $\Sigma^R_1$ are equal — since the initial states $\Sigma^I_0$ and $\Sigma^T_0$ differ only in their velocities.

The solution of the impact problem coincides with the solution of $RP_1$ up to the time $t_2 = t_1 + L/s^R_1$, where $s^R_1$ is the speed of the discontinuity $W^R_1$. At time $t = t_2$ the front $W^R_1$ reaches the free-surface located at $x_2 = x_1 + L$. To continue the solution of the impact problem beyond $t = t_2$, one needs to solve a second RP, $RP_2$ (which is marked 2 in Figure 1 (a)), centered at $(x_2, t_2)$ and characterized by the initial data $\Sigma^L_2 = \Sigma^R_1$ and $\Sigma^T_2 = \Sigma^V$. The solution to $RP_2$ consists of two austenitic states $\Sigma^L_2 = \Sigma^R_1$ and $\Sigma^T_2$, separated by 1-rarefaction discontinuity $W^J_2$, and of a vacuum state $\Sigma^T_2 = \Sigma^V$ separated from the austenite by a contact discontinuity $W^C_2$ at the monitored free surface.

**Regime B:** $u_f^{\text{crit}} < u_f < u_f^{\text{doub}}$. As we will see, Regime B is different from Regimes A and C: depending on the magnitude of the impact velocity $u_f$, three different sub-regimes may occur in this regime at the level of the third Riemann problem. These three sub-regimes differ qualitatively in the types of waves which are produced by the collision of a certain transformation front with a rarefaction wave resulting from reflection of the precursor shock.

Typical $(x, t)$-diagrams associated with sub-regimes B.1–B.3 are depicted in Figure 2; the particular data used to construct these graphs correspond to experiments number 1, 17, and 6.
Figure 1: \((x, t)\) diagrams for \(\alpha\)-\(\varepsilon\) phase transition in iron. (a) Regime A, (b) Regime C. Thick dashed lines denote fronts; grey lines denote shock fronts and black lines denote transformation fronts. Thick solid grey lines denote rarefaction waves. Thin solid black lines denote iron-vacuum interfaces. Thin dashed grey lines denote contact discontinuities between the same phases of iron. Note that all contact discontinuities are virtually degenerate: waves do not interact noticeably with them, and therefore the corresponding vanishingly weak waves produced by such interactions are not shown.

of (Barker & Hollenbach, 1974), respectively. These graphs give qualitatively identical results for RPs \(RP_1\) and \(RP_2\). As presented in Figure 2 (b), the solution to \(RP_1\) consists of four states \(\Sigma^I_0, \Sigma^L_1, \Sigma^R_1, \) and \(\Sigma^T_0\) separated by three waves \(W^L_1, W^C_1, \) and \(W^R_1\). The states \(\Sigma^I_0\) and \(\Sigma^T_0\) are the initial austenitic states while the states \(\Sigma^L_1, \Sigma^R_1\) are martensitic. \(W^L_1\) and \(W^R_1\) are split waves: \(W^R_1\) consists of a shock front \(W^{Ra}_1\) and a transformation front \(W^{Rb}_1\) separated by a critical austenitic state \(\Sigma^{crit}_1\). Similarly, \(W^L_1\) consists of a shock front \(W^{La}_1\) and a transformation front \(W^{Lb}_1\) separated by a critical austenitic state \(\Sigma^{Lcrit}_1\).

The solution of the impact problem coincides with the solution of \(RP_1\) up to time \(t_2 = t_1 + L/s^Ra_1\). At this time the front \(W^{Ra}_1\) reaches the free-surface located at \(x_2 = x_1 + L\). To continue the solution of the impact problem beyond \(t = t_2\) one needs to solve the second RP, \(RP_2\), which is centered at \((x_2, t_2)\) with initial data \(\Sigma^La_2 = \Sigma^{Rcrit}_1\) and \(\Sigma^{Ra}_2 = \Sigma^V\). The solution to \(RP_2\) consists of two austenitic states \(\Sigma^{Rcrit}_1\) and \(\Sigma^{Lb}_2\) and vacuum state \(\Sigma^V\). The austenitic states \(\Sigma^{Rcrit}_1\) and \(\Sigma^{Lb}_2\) are separated by a 1-rarefaction wave \(W^L_2\); the contact discontinuity \(W^C_2\) is the boundary between the state \(\Sigma^{Lb}_2\) and vacuum.

The structure of the solution of the impact problem changes again at time \(t_3 = (x_2 - x_1 + s^{Rb}_1, t_2 - s^{Rb}_L, t_1 - s^{L}_L)/(s^{Rb}_1 - s^{L}_L).\) At this time the transformation front \(W^{Rb}_1\) collides with the rarefaction wave \(W^L_2\) at point \(x_3 = (s^{Rb}_1, x_2 - s^{L}_L, t_2 - t_1)/(s^{Rb}_1 - s^{L}_L).\) Evaluation of the solution for times beyond \(t = t_3\) requires solution of a third RP, \(RP_3\), centered at \((x_3, t_3)\) with initial data \(\Sigma^La_3 = \Sigma^{Rb}_1\) and \(\Sigma^{Ra}_3 = \Sigma^{Lb}_2.\) As mentioned above the structure of the solution to \(RP_3\) depends on the magnitude of the impact velocity \(u_j\). From this point onwards...
three qualitatively different sub-regimes must be considered separately. In detail, we will show that there are two limiting speeds $u_{f12}$ and $u_{f23}$ which characterize three qualitatively different observable sub-regimes: Regime B.1, $u_{f,crit} < u_f < u_{f12}$; Regime B.2, $u_{f12} < u_f < u_{f23}$; and Regime B.3, $u_{f23} < u_f < u_{f, doubl}$; compare Section 4.1.

**Regime B.1:** $u_{f,crit} < u_f < u_{f12}$. In this sub-regime, after the compressive austenite-to-martensite transition front $W_1^{R,b}$ meets the rarefaction wave $W_2^{L}$ a “reverse-transformation tendency” prevails: the transition front $W_1^{R,b}$ is sufficiently weak for the reverse transformation — from martensite to austenite — to be initiated at $(x_3,t_3)$. For $t > t_3$ we have a right-facing compressive front $W_3^{R}$ in austenite and a left-facing rarefying split wave $W_3^{L}$ (composed of a rarefaction wave $W_3^{L,a}$ and a transformation front $W_3^{L,b}$) which transforms martensite back to austenite.

The solutions of three additional RPs — $RP_1$, $RP_3$, and $RP_6$ — are necessary to cover the time-range of the experimental profiles reported in (Barker & Hollenbach, 1974). $RP_3$ and $RP_6$ are very similar to $RP_2$; see Figure 2 (a) and (b). It is interesting to note, finally, that the wave interactions associated with the Riemann problem $RP_3$ result in acceleration of the back transformation front, and give rise to a right traveling shock wave which compensates for the resulting differences in stress.

**Regime B.2:** $u_{f12} < u_f < u_{f23}$. In this case, after the compressive transformation front $W_1^{R,b}$ meets the rarefaction wave $W_2^{L}$ the “direct” and “reverse” transformation tendencies balance each other. The transformation front $W_1^{R,b}$ is not sufficiently weak for the reverse transformation to occur (as it does in Regime B.1), nor it is large enough for the direct transformation to proceed further beyond the collision point $(x_3,t_3)$ — as is the case in the Regime B.3 described below. The collision gives rise to left-facing rarefaction wave $W_3^{L}$ in martensite and a right-facing shock front $W_3^{R}$ in austenite. The austenite and martensite regions are separated by a contact discontinuity $W_3^{C}$ which is not crossed by material particles: $W_3^{C}$ separates materials in two different phases, but no transformation processes take place in connection with this wave. (We notice that the size of the interval $u_{f12} \ldots u_{f23}$ in which Regime B.2 occurs is closely related to the size of the hysteresis of the material — iron in this specific case. In particular, if the material does not have any hysteresis at all, then $u_{f12} = u_{f23}$ and only two sub-regimes Regime B.1 and Regime B.3 remain.)

As in Regime B.1, solutions of three additional RPs — $RP_1$, $RP_3$, and $RP_6$ — are necessary to cover the time-range of the experimental profiles reported in (Barker & Hollenbach, 1974); the corresponding depictions given in Figure 2 (c) can be interpreted in a manner analogous to that of Regime B.1.

**Regime B.3:** $u_{f23} < u_f < u_{f, doubl}$. In this sub-regime, after $W_1^{R,b}$ meets $W_2^{L}$ the “direct-transformation tendency” prevails. The transformation front $W_1^{R,b}$ is sufficiently strong to sustain the direct transformation beyond the collision point $(x_3,t_3)$. In the solution to $RP_3$,
Figure 2: $(x, t)$ diagrams for $\alpha$-$\epsilon$ phase transition in iron for Regime B. (a) Regime B.1, (b) blowup of (a) showing details of the solutions of $RP_1 \ldots RP_4$, (c) Regime B.2, (d) Regime B.3. Thick dashed lines denote fronts: grey lines denote shock fronts and black lines denote transformation fronts. Thick solid grey lines denote rarefaction waves. Thin solid black lines denote iron-vacuum interfaces. Thin dashed lines denote contact discontinuities: grey lines denote contacts between the same phases of iron and black lines denote contacts between the different phases of iron. Note that all contact discontinuities are virtually degenerate: waves do not interact noticeably with them, and therefore the corresponding vanishingly weak waves produced by such interactions are not shown.
the left-facing wave $W^L_2$ is a rarefying wave in martensite and the right-facing wave $W^R_3$ is a compressive split wave (composed of a shock front $W^{Ra}_3$ and a transformation front $W^{Rb}_3$) which keeps on transforming austenite to martensite.

The solutions of RPs $RP_4$, $RP_5$, and $RP_6$ are depicted in Figure 2 (d) and can be interpreted in a manner analogous to that of Regime B.1.

**Regime C:** $u_f \geq u_{f,doub}$. A typical $(x, t)$-diagram is depicted in Figure 1 (b); the particular data used to produce this graph corresponds to experiment number 9 in (Barker & Hollenbach, 1974). As in Regime A, upon impact only one discontinuity propagates into the target and only one discontinuity propagates into the flyer. These compressive transformation fronts, which are labelled $W^R_1$ and $W^L_2$ in Figure 1 (b), are the only genuine discontinuities in the solution to $RP_1$; the III $W^C_1$ is a degenerate contact discontinuity: all flow quantities are continuous across this surface.

The second RP (problem $RP_2$ marked 2 in Figure 1 (b)) arises as the front $W^R_1$ reaches the free-surface. We point out that the left-facing wave $W^L_2$ is a rarefying split-wave — composed of a precursor rarefaction wave $W^{La}_2$ followed by a transformation front $W^{Lb}_2$.

### 3.2 Graphite–diamond phase transition

In the experiments presented in (Erskine & Nellis, 1992) the MI, which was again monitored by a VISAR, is not a free surface. Indeed, to minimize reflections at the MI, this configuration has the graphite specimen backed by a transparent LiF window — whose impedance is similar to that of graphite. In this section we describe the feasible flow regimes within the flyer-target-window system for the experiments of (Erskine & Nellis, 1992). The presentation here parallels that of Section 3.1 and only the relevant differences will be emphasized.

We begin by considering the initial configuration $\Sigma(x, t_1)$ of states at the impact time $t = t_1$ for which we use notations similar to those of (1):

$$\Sigma(x, t_1) = \begin{cases} 
\Sigma^I_0, & x < x_1 \\
\Sigma^T_0, & x_1 < x < x_1 + L \\
\Sigma^W_0, & x_1 + L < x .
\end{cases} \quad (2)$$

Here $\Sigma^I_0 = (v^G_0, 0, u_f)$ is the initial state of the copper impactor, $\Sigma^T_0 = (v^G_0, 0, 0)$ is the initial state of the graphite target and $\Sigma^W_0 = (v^G_0, 0, 0)$ is the initial state of the LiF window. The data (2) on the flyer-target-window system gives rise to $RP_1$. This RP is centered at $(x_1, t_1)$ with left state $\Sigma^La_1 = \Sigma^I_0$ and right state $\Sigma^{Ra}_1 = \Sigma^T_0$. The other RP arising from the data (2), which is centered at $(x_1 + L, t_1)$, has a trivial solution. (Similar to the case of iron presented in Section 3.1, in our modeling of the graphite-diamond transition experiments we assume semi-infinite impactors and windows. Again, we do not use finite-size impactors and windows.
since the sizes of the impactors and windows used are not provided in (Erskine & Nellis, 1992). The corrections to the computed observables that would result from the calculations utilizing finite-size impactors and windows are discussed in Section 4.1.)

Depending on the magnitude of the impact velocity $u_f$, $RP_1$ admits solutions of different types and thus, it gives rise to various flow regimes. As in Section 3.1, three qualitatively different flow regimes are to be distinguished. The initial stages (given by the solutions to $RP_1$s) in these regimes are very similar to those in the corresponding regimes of Section 3.1. The minor differences between the solutions to $RP_1$s considered in this section and those considered in Section 3.1 arise from the types of impactors used in associated experimental configurations. In particular, in the configuration considered presently, (i) the impactor and target are made of different materials and (ii) no phase transition occurs in the impactor. As a result, in the solution to $RP_1$ in each of the three flow regimes — presented in Figure 3, (i) the contact discontinuity $W^L_1$ is necessarily not degenerate and (ii) the left-facing wave $W^L_1$ is necessarily a single shock-front.

The differences between the latter stages (given by the solutions to $RP_2$, ...) of the flow resulting from the data (2) and those resulting from the data (1) turn out to be more substantial. These differences stem from the presence of a LiF window in the configuration corresponding to (2). In the rest of this section we discuss the latter stages of the flow resulting from the initial data (2). We note that to describe the main observables during the time-ranges of the experimental profiles reported in (Erskine & Nellis, 1992) it is sufficient to consider only one additional RP — $RP_2$ — in Regimes A and C and three additional RPs — $RP_2$, $RP_3$, and $RP_1$ — in Regime B. (The waves generated in some later RPs — $RP_5$, $RP_6$, ... in Regimes B and $RP_3$, $RP_1$, ... in Regimes C — will still reach the MI within the the time-ranges under consideration and have been fully taken into account in the our computations; see Section 4.2. The corrections to the observable MI velocity profiles due to arrival of these waves are rather weak, however, and an extended discussion of their character does not seem necessary at this point.)

Regime A: $u_f \leq u_{f,\text{crit}}$. A typical $(x,t)$-diagram is depicted in Figure 3 (a); none of the experiments of (Erskine & Nellis, 1992) corresponds to this regime. $RP_2$ arises as the shock front $W^R_1$ reaches the target-window interface. The solution to $RP_2$ has the following structure: the left states — $\Sigma^R_{1,b}$ and $\Sigma^L_{2,b}$ — are austenitic states and the right states — $\Sigma^R_{2,b}$ and $\Sigma^W_0$ — are LiF states; the left- and the right-facing waves — $W^L_2$ and $W^R_2$ — are single-shock fronts; finally, the contact discontinuity $W^L_1$, separating graphite and LiF, is the MI.

Regime B: $u_{f,\text{crit}} < u_f < u_{f,\text{doub}}$. A typical $(x,t)$-diagram is depicted in Figures 3 (c), (d); the particular data used to produce this graphs corresponds to experiment labeled gF in (Erskine & Nellis, 1992).

$RP_2$ results from the interaction of the front $W^R_1$ with the target-window interface. In the solution to $RP_2$, the left-facing wave $W^L_2$ is a transition front, transforming austenite to martensite, and the right-facing wave $W^R_2$ is a shock front transmitted into the LiF window. The next RP, $RP_3$, follows from the collision of two transformation fronts $W^R_1$ and $W^L_1$. The solution to $RP_3$ has the following structure: all four states — $\Sigma^R_{1,b}$, $\Sigma^L_{2,b}$, $\Sigma^R_{3,b}$, and $\Sigma^L_{3,b}$ — are
Figure 3: \((x, t)\) diagrams for graphite-diamond phase transition experiments. (a) Regime A, (b) Regime C, (c) Regime B, (d) blowup of (c) showing details of the solutions of \(RP_3\) and \(RP_4\). Thick dashed lines denote fronts; grey lines denote shock fronts and black lines denote transformation fronts. Thick solid grey lines denote rarefaction waves. Thin solid black lines denote interfaces between different materials: the interface between the impactor (copper) and the target (carbon) and the interface between the target (carbon) and the window (LiF). Thin dashed grey lines denote contact discontinuities between the same phases of carbon. Note that all contact discontinuities are virtually degenerate: waves do not interact noticeably with them, and therefore the corresponding vanishingly weak waves produced by such interactions are not shown.
<table>
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Table 1: Comparison of the experimental and computed values of the observables for $\alpha - \epsilon$ shock-induced phase transition in iron. The following observables are presented: $t_2$ and $t_3$ — times at which the major jumps in free-surface velocities take place and $W_2^C$ and $W_6^C$ — free-surface velocities. The experimental values of $t_2$ and $t_3$ were obtained as the midpoints of the relevant velocity increase intervals in Figure 4 left. Variables $t_2$, $t_3$, $W_2^C$ and $W_6^C$ are introduced in Section 3.1. Times are in s/km, velocities are in km/s.

martensitic and the left- and the right-facing waves — $W_3^L$ and $W_3^R$ — are shock fronts. Finally, $RP_4$ arises when the shock front $W_3^R$ reaches the target-window interface. In the solution to $RP_4$, the left-facing wave $W_4^L$ is a rarefaction wave reflected into the target and the right-facing wave $W_4^R$ is a shock front transmitted into the window.

**Regime C:** $u_f \geq u_{f,\text{doub}}$. A typical $(x, t)$-diagram is depicted in Figure 3 (b); the specific data used to produce this graph corresponds to experiment named gE in (Erskine & Nellis, 1992). $RP_2$ arises as the transformation front $W_4^R$ reaches the target-window interface. The solution to $RP_2$ in this regime has the same structure as that in Regime A with the only difference that, in the present regime, the left states — $\Sigma_1^{R,b}$ and $\Sigma_2^{L,b}$ — are martensitic.

## 4 Quantitative Predictions

### 4.1 $\alpha-\epsilon$ phase transition in iron

In this section we compare our predictions for phase transitions in iron with the corresponding results of experiment. Our calculations require EOSs data for the $\epsilon$ and $\alpha$ phases of iron together with critical negative normal stress curves; therefore, in this section we also include a discussion of the associated material parameters.

In Figure 4 we show free-surface velocity histories predicted by our model and those constructed from experimental data reported in (Barker & Hollenbach, 1974). These velocity histories fall within the various regimes discussed in Section 3.1: experiments 14, 1, 17, 6, and 9 correspond to Regimes A, B.1, B.2, B.3, and C, respectively. Comparison of theoretical curves (Figure 4, right) and experimental curves (Figure 4, left) shows very good qualitative and quantitative agreement, well within the margin expected from the uncertainties associated with the EOS we use — see also Table 1.
Figure 4: α–ε shock induced phase transition in iron. Left: Experimental curves (Barker & Hollenbach, 1974). Right: Predictions. Free-surface velocity profiles are presented for six experiments numbered according to (Barker & Hollenbach, 1974). The corresponding impactor velocities are: 14, 0.6127 km/s; 1, 0.9916 km/s; 17, 1.307 km/s; 6, 1.567 km/s; 9, 1.900 km/s. As in (Barker & Hollenbach, 1974), the time axes are normalized by dividing the actual time from impact by the specimen thickness.

Each free-surface velocity profile takes a form of a several-step staircase. These staircase-like shapes of free-surface velocity histories are due to front reflections, as explained in Section 3.1: each reflection of a front from the free surface results in a jump in a free-surface velocity. We note that while the computed profiles exhibit sharp velocity jumps, the experimental profiles feature more gradual velocity increases. The difference is due to the fact that in our model all shock waves and transformation fronts are represented by infinitely thin discontinuities; see Section 1 in Part I.

We should also notice two features of the experimental profiles which are absent from the theoretical profiles: (i) small steps located at \( t \approx 0.165 \) s/km and (ii) additional changes in the free-surface velocities which begin at \( t \approx 0.5 \) s/km. The small step (i) on an experimental profile is caused by the arrival of an elastic precursor wave (Barker & Hollenbach, 1974) at the free-surface. Since our EOS for α-iron does not account for elastic effects these small increases in the surface velocities are absent from the computed profiles. As argued in (Barker & Hollenbach, 1974), in turn, the changes (ii) in the free-surface velocity, are due to the arrival of a rarefaction wave that originates either from lateral edge effects (which are not taken into account in this one-dimensional infinite-plate model) or from reflection of a front from the back surface of the impactor (which is an iron-aluminum interface). It should be possible to capture all such experimental features if a fully three-dimensional shock-capturing numerical scheme is used (Weatherwax et al., 2000).
In the rest of this section we discuss the material parameters needed for the EOS and critical curves of iron — whose general forms are given in the Appendix. We first note that the iron used in the experiments is a polycrystalline material in which the component crystallites are randomly oriented. As a result, on the macroscopic level, both \( \alpha \)- and \( \varepsilon \)-iron behave as isotropic solids (although each individual crystallite, on the microscopic level, possesses higher symmetry: \( \alpha \)-iron has the body-centered cubic structure and \( \varepsilon \)-iron has the hexagonal close-packed structure). Furthermore, the magnitude of the stresses involved is far beyond the yield stress of \( \alpha \)-iron: For tensile tests performed at a nominal strain rate of \( 1.7 \times 10^{-4} \text{s}^{-1} \) in (Kuramoto et al., 1979), for example, the yield stress is less than 0.1 GPa; the yield stress corresponding to an elastic precursor reported in (Barker & Hollenbach, 1974), in turn, is \( \sim 1 \) GPa. Thus, anisotropy and non-hydrostatic effects can safely be neglected in the high stress experiments considered presently, see also (Duvall & Graham, 1977; Al'tshuler, 1978; Davison & Graham, 1979; Brown & McQueen, 1986). In particular, the tensor of Grüneisen parameters can be assumed isotropic \( \gamma_{ij} = \delta_{ij} \gamma \), and the stress state can be assumed hydrostatic, \( q = p \).

A great deal of uncertainty exists with regards to \( \alpha - \varepsilon \) critical pressure curves (4); see e.g. (Huang et al., 1987; Manghnani et al., 1987; Besson & Nicol, 1990; von Bargen & Boehler, 1990): values of room-temperature forward-transformation pressures \( \tilde{q}_{F0} \) have been report-
ed within the range of 9...15 GPa, while those for backward-transformation lie within the range of 7...10 GPa. The reported values of the forward-transformation slope \( \frac{\tilde{q}}{d\tilde{\theta}}|_{F0} \), in turn, vary from \(-0.0059 \text{ GPa/K} \) to \(0.0022 \text{ GPa/K} \). No reliable measurements of the backward-transformation slope \( \frac{\tilde{q}}{d\tilde{\theta}}|_{B0} \) exist to our knowledge; however, it is reasonable to assume that \( \frac{\tilde{q}}{d\tilde{\theta}}|_{B0} \) is of the same order of magnitude as \( \frac{\tilde{q}}{d\tilde{\theta}}|_{F0} \).

For both \( \alpha \)- and \( \varepsilon \)-iron EOSs we utilize Mic-Grüneisen equations of the type presented in the Appendix. As reference curves we use the first and third sub-branches of a single well-documented (Marsh, 1980; Barker, 1975) front-curve for the \( \alpha \) and \( \varepsilon \) phases of iron respectively, as indicated in the Appendix. This reference curve is centered at the austenitic standard state \( \Sigma^0_r = (u^0_r, q^0_r, u^0_s) = (u^0_s, 0, 0) \) with \( u^0_s = 0.127 \text{ cm}^3/\text{g} \). The projection of the reference curve for \( \alpha \)-iron onto the \((u, s)\)-plane is well approximated by a straight line (11) with \( a^0_r = 4.63 \text{ km/s} \) and \( b^0_r = 1.33 \) (Barker, 1975). There is no definitive parameterization of the reference curve, in the case of the \( \varepsilon \)-iron, however: three sets of parameters for the \( \varepsilon \)-iron reference curve (17) have been widely used in the literature (McQueen et al., 1970; Al'tshuler et al., 1981; Brown & McQueen, 1986). However, these parameters are based on data in a large range of velocities \( u^0_r \), spanning regions which also include the \( \gamma \) and even liquid phases of iron; see e.g. (Brown & McQueen, 1986; Anderson & Ahrens, 1994). To avoid possible systematic errors arising from use of experimental points pertaining to liquid and \( \gamma \)-iron data, we fit (17) to the data from that portion of the reference front-curve that falls in the \( \varepsilon \)-iron region only. (The boundary of the \( \varepsilon \)-iron region was estimated in (Brown & McQueen, 1986)). In detail, we used the \((u, s)\)-data from (Marsh, 1980) for which \( u \) falls between 0.763 km/s and 2.0 km/s; we excluded the lowest particle velocity point, 0.573 km/s, from the fit because it seems to fall away from the trend established by the rest of the data. The resulting fit yields \( a^0_r = 3.2 \text{ km/s}, b^0_r = 2.3, \) and \( c^0_r = -0.2 \text{ s/km} \). This set of parameters corresponds to the choices \((u^0_r, s^0_r) = (0.763, 4.913), s^0_{r,1} = 2.07 \) and \( s^0_{r,2} = -0.09 \) in equation (17).
As for the Grüneisen coefficient for α-iron, the value of the parameter $\gamma_r^{b,0} = 1.66 \ldots 1.69$ in (16) (which gives the Grüneisen parameter under standard conditions) is well known (McQueen et al., 1970; Ramakrishnan et al., 1978); reference (Ramakrishnan et al., 1978), in turn, gives the value $g_r^{b,0} = 1.0$ for the $g$-parameter in (16). Unfortunately, there is no conclusive experimental data on the specific volume dependence of the Grüneisen parameter for ε-iron. We evaluated the $\gamma_r^{b,0}$ and $g_r^{b,0}$ parameters of equation (16) using $v_r^{b,0} = v_r^0 (1 - v_r^{b,0}/s_r^0) = 0.108 \text{ cm}^3/\text{g}$ and various types of $\gamma = \gamma(v)$ dependencies found in the literature — as we describe in what follows. Grüneisen parameter estimates based on finite differences in thermal pressure between porous and non-porous shock-compression data were reported in (McQueen et al., 1970); the same data was later reconsidered in (Jeanloz, 1979). For $\gamma = \gamma(v)$ dependencies obtained in (McQueen et al., 1970) and (Jeanloz, 1979) we get $\gamma_r^{b,0} = 1.4$, $g_r^{b,0} = 1.4$ and $\gamma_r^{b,0} = 1.8$, $g_r^{b,0} = 3.0$, respectively. Other estimates of the dependence $\gamma = \gamma(v)$, based on combinations of experimental data and theoretical calculations, was reported in (Grover, 1990). For these dependencies we get $\gamma_r^{b,0} = 1.9$, $g_r^{b,0} = 0.8$ (model A of (Grover, 1990)) and $\gamma_r^{b,0} = 1.7$, $g_r^{b,0} = 0.8$ (model B of (Grover, 1990)).

As we can see, large uncertainties exist in defining the critical pressure curves and the dependence of the Grüneisen parameter on the specific volume. To resolve this problem, we tested various combinations of the coefficients in (4) and (16). As a result of these calculations we concluded that: (i) The variations in the values obtained from experiment for the coefficients in (16) and for the slopes in both equations (4) do not substantially influence our predictions for shock experiments. (ii) Out of the range of values $7 \leq \bar{q}_{F0} \leq 10$ reported in the literature, the value $\bar{q}_{F0} = 9 \text{ GPa}$ gives a good agreement with all sixteen experiments of (Barker & Hollenbach, 1974) we consider. (iii) The results of the simulations are sensitive to the choice of $\bar{q}_{F0}$; the best agreement with the experimental results was achieved for $\bar{q}_{F0} = 13 \text{ GPa}$. In sum, in the computations presented in this paper, we used $\bar{q}_{F0} = 13 \text{ GPa}$ and $\bar{q}_{F0} = 9 \text{ GPa}$, and we set both slopes $\partial q / \partial \theta$ in (4) to zero. This estimates lead to predictions whose distance to all experimental measurements lies within the overall experimental uncertainty.

### 4.2 Graphite–diamond phase transition

We now turn to the graphite–diamond transition. As in the previous section, we compare the predicted profiles to those obtained experimentally, and we discuss the material parameters needed for the EOS and critical curves.

In Figure 5 we show velocity histories for the MI as predicted by our model together with those constructed from experimental data reported in (Erskine & Nellis, 1992). These velocity histories fall within two of the regimes discussed in Section 3.2: experiments with impact velocities 2.60, 3.12, and 3.47 km/s lie within Regime B, whereas the experiment with impact velocity 3.90 km/s corresponds to Regime C. Comparison of theoretical curves (Figure 5, right) and experimental curves (Figure 5, left) shows good qualitative and quantitative agreement, again, within the margin expected from the uncertainties associated with the rough form of the EOS we use — see also Table 2. The MI velocity profiles depicted in Figure 5 are similar to
Figure 5: Graphite–diamond shock induced transformation experiments. Left: Experimental curves (Erskine & Nellis, 1992). Right: Predictions. MI velocity profiles are presented for four experiments labeled according to (Erskine & Nellis, 1992). The corresponding impactor velocities are: \(gF\), 2.60 km/s; \(gG\), 3.12 km/s; \(gD\), 3.47 km/s; \(gE\), 3.90 km/s. As in (Erskine & Nellis, 1992), the curves are staggered horizontally on the graphs for clarity.

those presented in Figure 4: each MI velocity profile takes a form of a several-step staircase, and while the computed profiles exhibit sharp velocity jumps, the experimental profiles feature somewhat more gradual velocity increases. We point out that the small steps present in the computed profiles are due to the arrival at the MI of weak waves mentioned in Section 3.2.

In the remainder of this section we discuss the material parameters needed for the EOS and critical curves — whose general forms are given in the Appendix. The target material used in the experiments considered in this section was (highly oriented) pyrolytic graphite — in which \(c\) axes of the component crystallites are nearly parallel to the impact velocity vector. Unlike the case of iron, we may not assume in this case that stresses are hydrostatic — since (i) Graphite does not exhibit any noticeable plastic behavior, and (ii) Highly oriented polycrystalline graphite, as well as single-crystal graphite, is strongly anisotropic.

(The anisotropic character of single crystalline hexagonal graphite is well understood: it arises as a result of the layered atomic structure of this material — with layers normal to the \(c\) direction. Carbon atoms within the layers are connected by strong \(sp^2\)-type covalent bonds while the bond between layers has the nature of a weak van der Waals force. Consequently, compressibility along the \(c\)-axis is much larger than that along the \(a\)-axis; furthermore, the transformation of graphite under high pressure and at relatively low temperature is mostly controlled by the component \(q\) of the stress in the direction of the \(c\) axes.)

A wide range of EOS data for graphite-to-diamond phase changes has been put forward in
Table 2: Comparison of the experimental and computed values of the observables for graphite-diamond shock induced transformation. The following observables are presented: $t_2$ and $t_4$ — times at which the major jumps in MI velocities take place and $W^C_2$ and $W^C_4$ — MI velocities. The experimental values of $t_2$ and $t_4$ were obtained as the midpoints of the relevant velocity increase intervals in Figure 5 left. Variables $t_2$, $t_4$, $W^C_2$ and $W^C_4$ are introduced in Section 3.2. Times are in ms, velocities are in km/s.

the last four decades, including static compression data (Bundy & Kasper, 1967; Goncharov et al., 1989; Hanfland et al., 1989a; Zhao & Spain, 1989; Hanfland et al., 1989b; Goncharov, 1990b; Goncharov, 1990a; Takano et al., 1991; Utsumi & Yagi, 1991b; Yagi et al., 1992) as well as shock compression data (Doran, 1963; Coleburn, 1964; Marsh, 1980; Gust, 1980; Erskine & Nellis, 1991; Erskine & Nellis, 1992). In addition to this experimental work, several groups performed theoretical first-principles calculations of the structure and the physical properties of graphite and its high-stress phases (Fahy et al., 1986; Fahy et al., 1987; Fahy & Louie, 1987; Boettger, 1997; Wu & Xu, 1998; Wu & Xu, 1999). Although the changes in structure and the physical properties accompanying cool compression of graphite are still not fully understood, a number of facts may be ascertained from these experiments and calculations, as discussed in what follows.

The most thorough and exhaustive study of stress-induced phase transformation for single-crystal and highly-oriented polycrystalline graphite was reported by Utsumi and Yagi et al (Utsumi & Yagi, 1991b; Utsumi & Yagi, 1991a; Yagi et al., 1992). The following properties of the transition and the high-stress phase were observed in these quasi-static, room-temperature compression experiments:

1. In quasi-hydrostatic environments, the transition starts and is completed in a very narrow pressure interval between 18 and 19 GPa. These values were corroborated in (Goncharov et al., 1989; Goncharov, 1990b; Goncharov, 1990a; Takano et al., 1991) where the value of transition pressure for single crystal or highly-oriented polycrystal under hydrostatic loading was reported within the range of 18...23 GPa.

2. The transition is reversible but has a very large hysteresis — backward transformation occurs at 2...5 GPa. The similar range of the backward-transformation pressures was corroborated in (Goncharov et al., 1989; Takano et al., 1991), and the range of 5...8 GPa was reported (Bundy & Kasper, 1967).

3. X-ray-diffraction profiles obtained on the high-stress phase are consistent with the hexag-
4. The observed orientation relationship between the graphite and high-stress hexagonal diamond phase is consistent with the martensitic transition mechanism proposed in (Bundy & Kasper, 1967; Lonsdale, 1971).

A rationale — clearly supported by experiment — was offered in (Yagi et al., 1992) to explain the substantial scatter in the values of transition pressure reported in the literature: The value of the transition pressure is very sensitive to (i) The configuration of stresses occurring in the experiment and (ii) The degree of the orientation of the crystallites of the polycrystalline graphite. In particular, it was suggested in (Yagi et al., 1992) that the deviation from hydrostatic compression explains the lower transformation pressure values reported in (Bundy & Kasper, 1967; Hanfland et al., 1989b; Goncharov, 1990a; Yagi et al., 1992) and that insufficient order of crystallites accounts for the elevated transition pressure values observed in (Bundy & Kasper, 1967; Coleburn, 1964; Gust, 1980; Marsh, 1980; Goncharov, 1990a; Erskine & Nellis, 1992; Yagi et al., 1992).

The lower transformation pressures, in the range of 14...16 GPa, were observed (Bundy & Kasper, 1967; Hanfland et al., 1989b; Goncharov, 1990a; Yagi et al., 1992) in the experiments in which the highly-oriented graphite specimens were compressed, predominantly in the c-axis direction, in a solid pressure-transmitting medium. Since the most important factor for the onset of the transition is the stress component \( q \) along the c axis, the reduction of the nominal transformation pressures may be attributed to non-hydrostatic conditions of loading \( (p < q) \), a heterogeneous compression — some portion of the sample may be compressed more than the average, and/or different calibrating scales used to determine the pressure.

The higher transformation pressures, on the other hand, were observed in several static and dynamic compression studies — 23 GPa in (Yagi et al., 1992) in Drickamer-type anvil, 34 GPa in (Gust, 1980), 44 GPa in (Goncharov, 1990a), 45 GPa in (Marsh, 1980), 25...45 Gpa (Erskine & Nellis, 1992), no transition was observed up to 50 GPa in (Coleburn, 1964), no transition was observed up to 18 GPa in (Yagi et al., 1992) in cubic anvil apparatus, no transition was observed in (Bundy & Kasper, 1967) — in which specimens of poorly oriented polycrystalline graphite were used. It was argued in (Yagi et al., 1992; Erskine & Nellis, 1992) that since the transition has a martensitic nature, the relative orientation of adjacent atomic layers in different crystallites is very important. A slightly different explanation of the elevated values of the transition pressure for poorly oriented polycrystalline graphite was offered in (Bundy & Kasper, 1967): large transition pressures were interpreted there as a result of the strong directional dependence of the mechanical properties and behavior of a single crystallite. In detail, as mentioned earlier, a single crystal of graphite is very strong and relatively incompressible in any direction perpendicular to the c axis. This suggests that in poorly oriented polycrystalline graphite specimens the crystallites most susceptible to an imposed predominantly uniaxial compression would be those with their c axes roughly parallel to the axis of compression. The other crystallites would resist compression and would deform mainly by bending or buckling. “Arches” of these “edgewise” crystallites would tend to shield enclosed “flatwise” crystallites from the overall compressive action.
A variety of speculations can be found in the literature concerning a possible non-hexagonal atomic structure of the high-stress phase. In particular, it has been hypothesized that the martensitic phase could be an $sp^3$-bonded structure (Bundy & Kasper, 1967), an amorphous phase (Goncharov et al., 1989), or an intermediate phase between graphite and hexagonal diamond (Takano et al., 1991). A detailed discussion was presented in (Yagi et al., 1992) concerning these varied interpretations and, in particular, a critique was offered of the previous attempts to determine the crystal structure of the high-stress phase by x-ray diffraction.

Based on the discussion above we now turn to determining the material parameters needed for the EOS and critical curves. Due to strong anisotropy the transition is controlled mainly by the component $q = -\tau_{11}$ of the stress which is parallel to the $c$ axis; thus, as the first order approximation, we may disregard the influence of other stress components $\tau_{22}, \tau_{12}, \ldots$, see (Yagi et al., 1992). This allows us to use the transformation-stress data obtained from hydrostatic experiments for our uniaxial-strain configurations. In view of the discussion above and consistent with (Utsumi & Yagi, 1991b; Utsumi & Yagi, 1991a; Yagi et al., 1992) we assume forward-transition stress of $q_f$ 18 GPa. The quoted values of the transition pressure were obtained under room temperature experiments; the value $q_f$ 18 GPa we assume in our calculations, with no temperature dependence, leads us to predictions in agreement with the experiments of (Erskine & Nellis, 1991; Erskine & Nellis, 1992). Thus, it is reasonable to assume that the temperature increases in these experiments, which has been estimated to be of the order of 100K, does not give rise to radical changes in the value of the transition stress.

(Non of the experiments we consider require knowledge of the backward-transition stress $q_b$, on the other hand. Indeed, the only rarefaction wave which appears in our calculations for graphite is the wave $W_4^L$ described in Section 3.2. This wave releases the stress in martensite to a level which is much higher than any value of $q_b$ from the range of 2...5 GPa cited in (Utsumi & Yagi, 1991b; Utsumi & Yagi, 1991a; Yagi et al., 1992); thus exact values of the backward transformation stress are not necessary in the experiments we consider.)

For both graphite and hexagonal diamond EOSs we utilize Mie-Grüneisen equations of the type presented in the Appendix. In particular, we use the front-curve centered in the austenitic standard state $\Sigma_r = (v_r, q_r, u_r) = (v_r^g, 0, 0)$ (where $v_r^g = 0.443 \text{ cm}^3/\text{g}$) as reference curves for both EOSs. The reference curve for graphite was compiled from dynamic (Doran, 1963; Coleburn, 1964; Marsh, 1980; Gust, 1980) and static (Hanfland et al., 1989a; Zhao & Spain, 1989; Utsumi & Yagi, 1991a; Yagi et al., 1992) data. In particular, use of the Grüneisen parameter below allowed us to utilize isothermal data to obtain data for the reference shock-front curve. The values of $a^0$ and $b^0$ obtained from these two groups of experiments are in fairly good agreement: $a^0 = 4.0 \text{ km/s}$ and $b^0 = 2.2...2.3$ for the shock-compression experiments and $b^0 = 2.3...2.6$ for the static-compression experiments. Since the graphite used in static experiment was highly-oriented and the graphite used in dynamic experiments was poorly oriented, the agreement in the values of $a^0$ and $b^0$ suggests that the elastic properties of polycrystalline graphite are less sensitive to the degree of orientation of the crystallites than the transformation stress. In the numerical simulations presented here we assume $a^0 = 4.0 \text{ km/s}$, $b^0 = 2.6$ — the values corresponding to the most oriented graphite.
There is limited quantitative EOS data available for hexagonal diamond; the most complete and accurate data seems to be that of (Utsumi & Yagi, 1991a; Yagi et al., 1992). In that work the d-spacing parameters of hexagonal diamond as functions of applied pressure were measured. The sample was under predominantly uniaxial loading with the applied stress parallel to the c direction. From this data we approximate a uniaxial isothermal EOS for hexagonal diamond by the linear elasticity equation

\[ q = \tilde{K}_d (\eta - \eta_d) + \ldots, \]  

where \( \eta = 1 - v/\nu_0 \), with \( \eta_d = 0.35 \) and \( \tilde{K}_d \) in the range 1520…2150 GPa. We see that there is a large uncertainty in the value of \( \tilde{K}_d \). In the numerical simulations presented here we assume \( \tilde{K}_d = 1520 \) GPa, which leads to the best agreement with experiment. This choice, together with the use of the Grüneisen parameter below, translates into the following values for the parameters of the reference curve (17): \( a_r^0 = 0.6 \) km/s, \( b_r^0 = 2.4 \), and \( c_r^0 = 0.0 \) s/km.

Since graphite and hexagonal diamond are highly anisotropic, the various components of the tensor of Grüneisen parameters \( \gamma_{ij} \) have different values. In fact, for hexagonal crystals, the tensor \( \gamma_{ij} \) has only two independent non-zero components (Barron & Munn, 1967): \( \gamma_c \) and \( \gamma_a \) — in the directions parallel and perpendicular to the c axis, respectively. Thus, in our uniaxial-strain computations we must take \( \gamma = \gamma_c \) for graphite and \( \gamma = \gamma_a \) for diamond. Indeed, in the experiments under consideration, the uniaxial-strain direction coincides with the c direction of graphite and is normal to the c direction of the hexagonal diamond; see (Bundy & Kasper, 1967; Lonsdale, 1971) for orientation relationships for transitions between graphite and hexagonal diamond.

The value of the Grüneisen parameter under standard conditions \( \gamma_r^{b,0} = 0.35 \ldots 0.4 \) was calculated in (Bailey & Yates, 1970; Gauster & Fritz, 1974) from the measured values of the expansion coefficient, the specific heat, and the elastic moduli. The dependence of the Grüneisen parameter on the specific volume, however, is not well established. Linear volume dependence was suggested in (Grover, 1979) and (Gust, 1980) with \( \gamma_r^{b,0} = 0.35 \), \( g_r^{b,0} = -0.15 \) and \( \gamma_r^{b,0} = 0.4 \), \( g_r^{b,0} = -0.6 \), respectively. A rather complicated form of the volume dependence, on the other hand, was proposed in (van Thiel & See, 1989); when expanded in powers of \( \eta = 1 - v/\nu_0 \) around \( \eta = 0 \) this dependence yields \( \gamma_r^{b,0} = 0.36 \) and a positive value \( g_r^{b,0} = 0.43 \). In our model EOS we thus use \( \gamma_r^{b,0} = 0.4 \) and \( g_r^{b,0} = 0 \).

To our knowledge no measurements of the Grüneisen parameter of hexagonal diamond have been reported in the literature. In the absence of reliable experimental measurements, we turn to the theoretical first-principles study (Wu & Xu, 1999), from which the Grüneisen parameter can be estimated as close to 1. Another possibility is to assume the volume dependence of the Grüneisen parameter of hexagonal diamond is similar to that of cubic diamond. Various studies of cubic diamond report the interval of 0.6…1.5 for the Grüneisen parameter under standard conditions (with \( \nu_0 = 0.285 \)) and indicate increase of the Grüneisen parameter with the specific volume. (The value of the Grüneisen parameter under standard conditions \( \gamma_r^{b,0} = 0.6 \ldots 0.8 \) was calculated in (Parsons, 1977; Reber & Wang, 1996) from the measured values of the expansion coefficient, the specific heat, and the elastic moduli. Grüneisen parameter estimates based on differences in thermal pressure between porous and non-porous shock-compression data were
reported in (Pavlovskii, 1971) and lead to $\gamma_r^{b,0} = 0.9$ and $g_r^{b,0} = 2.4$. Linear volume dependence was proposed in (Gust, 1980) and (van Thiel & Ree, 1989) with $\gamma_r^{b,0} = 1.5$, $g_r^{b,0} = 0.5$ and $\gamma_r^{h,0} = 1.15$, $g_r^{h,0} = 1.15$, respectively.) Here we assume the values $\gamma_r^{b,0} = 1$ and $g_r^{b,0} = 0$ for hexagonal diamond.

Finally, to model the experiments reported in (Erskine & Nellis, 1992) it is necessary to utilize the EOSs for the flyer and window materials: copper and LiF. As in the case of iron, anisotropic and non-hydrostatic effects can safely be neglected for these materials (Duvall & Graham, 1977; Aftshuler, 1978; Davison & Graham, 1979; Brown & McQueen, 1986); thus, the tensor of Grüneisen parameters can be assumed isotropic $\gamma_{ij} = \delta_{ij} \gamma$ and the stress state can be assumed hydrostatic, $q = p$. Shock-front curves centered at the standard states $\Sigma_r = (v_r^o, q_r^o, u_r^o) = (v_s, 0, 0)$ (where $v_s = 0.112 \text{ cm}^3/\text{g}$ for copper and $v_s = 0.379\sigma_0 \text{ cm}^3/\text{g}$ for LiF) are readily available in the literature. Thus we shall use these shock-front curves as reference curves for the EOSs. The reference shock-front curves of copper and LiF are well approximated by a straight lines (11) with $a_r^0 = 3.91 \text{ km/s}$ and $b_r^0 = 1.51$ (Marsh, 1980) and $a_r^0 = 5.15 \text{ km/s}$ and $b_r^0 = 1.35$ (Marsh, 1980), respectively. In the calculations presented in Section 3.2 the only data required for copper is the reference shock-front curve. For LiF, on the other hand, in addition to the reference curve it is necessary to know the volume dependence of the Grüneisen parameter. The value of the Grüneisen parameter under standard conditions $\gamma_r^{b,0} = 1.63$ was obtained in (McLean & Smith, 1972), and the value of $g_r^{b,0} = 2.9$ was estimated from the data reported in (Rao, 1975).

### A Equations of State

Naturally, quantitative predictions follow from our model only after explicit constitutive relations of the type (I-20) and (I-21) are used. The results presented in this paper were derived by assuming some of the simplest approximations of the material properties: the well accepted linear dependence for either critical-stress curve (I-20)

$$ q = \tilde{q}_F (\theta) \equiv \tilde{q}_{F0} + \frac{dq}{d\theta} \bigg|_{F0} (\theta - \theta_0) \quad \text{and} \quad q = \tilde{q}_B (\theta) \equiv \tilde{q}_{B0} + \frac{dq}{d\theta} \bigg|_{B0} (\theta - \theta_0), \quad (4) $$

together with a Mie-Grüneisen EOS for either phase.
A.1 EOS for Pure Phases

The thermodynamic properties of a pure phase are completely determined by its specific internal energy $U$. In the uniaxial strain case the specific energy is a function of two variables, the specific volume $v$ and the specific entropy $S$: $U = \bar{U}(v, S)$; consequently, the negative normal stress $q = \bar{q}(v, S)$ and the temperature $\theta = \bar{\theta}(v, S)$ are given as first derivatives of $\bar{U}$

$$
\bar{q}(v, S) = -\frac{\partial \bar{U}}{\partial v}
\quad \text{and} \quad
\bar{\theta}(v, S) = \frac{\partial \bar{U}}{\partial S}
,$$

see Section 3 of Part I. The conservation laws (I-15) and (I-16) only require EOS data in the form of a relation $q = \bar{q}(v, U)$. Such a relation, which is often called an incomplete EOS (Menikoff & Plohr, 1988), can be determined from the complete EOS $U = \bar{U}(v, S)$ — by solving the latter for $S = S(v, U)$ and substituting for $S$ in $q = \bar{q}(v, S)$ — if the complete EOS is known. In our case, however, it is appropriate to use approximations for $q = \bar{q}(v, U)$ as obtained directly from experimental results.

A well accepted method to obtain such an approximation (Menikoff & Plohr, 1988) is based on use of an appropriately chosen reference wave curve, and a Taylor expansion of $\bar{q}(v, U)$ in the variable $U$ around this curve. In detail, using the projection $U = U^b_r(v)$ of this reference wave curve onto the $(U, v)$ plane we write

$$
\bar{q}(v, U) = \bar{q}(v, U^b_r(v)) + \frac{\partial \bar{q}}{\partial U} (v, U^b_r(v)) (U - U^b_r(v)) + \frac{1}{2} \frac{\partial^2 \bar{q}}{\partial U^2} (v, U^b_r(v)) (U - U^b_r(v))^2 + \ldots
$$

This expansion yields a sequence of approximations to the incomplete EOS.

The first order approximation is known as a Mie-Grüneisen EOS (Rice et al., 1958; Zel'dovich & Raizer, 1967; McQueen et al., 1970):

$$
\bar{q}(v, U) = q^b_r(v) + \frac{\gamma^b_r(v)}{v} (U - U^b_r(v))
.$$

Here

$$
\gamma \equiv v \frac{\partial \bar{q}}{\partial U}
\quad \text{and} \quad
\gamma_{11}
$$

23
denotes the component of the tensor of Grüneisen parameters in the $x$-direction. (A general tensor of Grüneisen parameters defined as

$$
\gamma_{ij} = -v \frac{\partial \tau_{ij}}{\partial U} = \left. -\frac{1}{\theta} \frac{\partial^2 U}{\partial S \partial E_{mn}} \right|_{E_m} F_{im} F_{jn}
$$

is discussed in (Plohr & Sharp, 1988.). As shown in Section 4, there is substantial uncertainty with regards to the numerical value of the Grüneisen parameter in the cases we consider — especially for martensitic phases. Fortunately, these uncertainties are of little consequence in our context, since our predictions turned out to be rather insensitive to the particular values used. (In fact this insensitivity justifies using the zeroth order approximation: the errors in our results are estimated by the small corrections which would result from use of various experimental values of the Grüneisen parameter; see Section 4.)

The zeroth order approximation gives the normal stress $q$ as a function of the specific volume $v$ only:

$$
\dot{q}(v, U) = q_r(v).
$$

This approximation effectively decouples the first two (mechanical) equations in (I-15) from the last (thermodynamic) equation: under this approximation the first two conservation laws only contain the unknowns $(v, u)$. Once this pair is found, using $q$ from (10), the unknown $U$ results from the third equation in (I-15).

**Remark 2** The zeroth order approximation has a direct consequence for the structure of the Riemann problem: it implies that a non-vanishing 2-wave (a contact discontinuity) can only be present in the solution of a Riemann problem when the initial states $\Sigma^{L,a}$ and $\Sigma^{R,a}$ belong to different materials or to different phases of the same material. In other words, when the initial states $\Sigma^{L,a}$ and $\Sigma^{R,a}$ belong to the same phase of the same material, the zeroth order approximation implies that the contact discontinuity in the corresponding solution of the Riemann problem actually vanishes and only two waves are left in the solution. Thus, the solution of such a Riemann problem consists of three constant states only — which are separated by left- and right-facing waves.

**Remark 3** The following physical justification was given in (Zel’dovich & Raizer, 1967) to the first and zeroth order approximations: since the thermal energy of the material compressed by relatively weak shocks is small, essentially all of the internal energy acquired by the medium from the wave is used to overcome the repulsive forces due to the compression and is stored in the form of potential elastic energy.

Next, we need to specify the reference curve. For both phases we use as reference curve the compressive portion of the wave curve for which the ahead state $\Sigma^a$ is the * austenitic * standard state — that is, the austenite at zero velocity $u^a = 0$, at zero normal stress $q^a = 0$, and with
specific volume $u_r^a$ as measured at room temperature. (The choice of this particular reference
curve is commonly made since its ahead state is the state from which wave curves are most
often determined in experiments (Rice et al., 1958; McQueen et al., 1970; Marsh, 1980). We
note that the reference curve for the austenite coincides with the first compression sub-branch
of the $\Sigma^a_r$-centered wave curve (see Section 4.2.1 of Part I; accordingly, the reference curve for
the martensite coincides with the third compression sub-branch of the same wave curve.)

Both of these sub-branches are specified by simple analytical formulae — which can be
obtained as follows. First, the projection of a sub-branch onto the $(u, s)$-plane is approximated
in the vicinity of a point $(u_r^{b,0}, s_r^{0})$ — which is the $(u, s)$-plane projection of a certain state $\Sigma_r^{b,0}$
— by its tangent:

$$s = s_r^{0} + s_{r,1}^0 (u_r^{b,0} - u_r^{b,0}) = a_r^0 + b_r^{0} u_r^{b,0}.$$  \hspace{1cm} (11)

Then, substitution of equation (11) into (I-16), introduction of the compression

$$\eta_r^{a,b} = 1 - \eta_r^{a,b} / \eta_r^{a} ,$$  \hspace{1cm} (12)

and elimination of the velocity $u_r^{b,0}$ leads to a system which describes the locus of thermodynamic
states along the sub-branch:

$$q_r^{b} (\eta_r^{a,b}, \Sigma_r^{a}, \Sigma_r^{b,0}) = q_r^{a} + \frac{\eta_r^{a,b}}{\eta_r^{a}} s^2 (\eta_r^{a,b}, \Sigma_r^{a}, \Sigma_r^{b,0}) ,$$  \hspace{1cm} (13)

$$U_r^{b} (\eta_r^{a,b}, \Sigma_r^{a}, \Sigma_r^{b,0}) = U_r^{a} + q_r^{a} u_r^{a} \eta_r^{a,b} + \frac{\eta_r^{a,b}^2}{2} s^2 (\eta_r^{a,b}, \Sigma_r^{a}, \Sigma_r^{b,0}) ,$$  \hspace{1cm} (14)

where

$$s^2 (\eta_r^{a,b}, \Sigma_r^{a}, \Sigma_r^{b,0}) = \frac{(a_r^0)^2}{1 - b_r^{0} \eta_r^{a,b}} .$$  \hspace{1cm} (15)

Finally, the dependence of the Grüneisen parameter on the specific volume is approximated as

$$\gamma_r^{b} (u_r^{b,0}) = \gamma_r^{b,0} \left( \frac{u_r^{b,0}}{u_r^{b,0}} \right) \gamma_r^{b,0} = \gamma_r^{b,0} - g_r^{b,0} \left( 1 - \frac{u_r^{b,0}}{u_r^{b,0}} \right) + \ldots ,$$  \hspace{1cm} (16)

where $\gamma_r^{b,0}$ and $g_r^{b,0}$ are material constants. We note that for either sub-branch, the state $\Sigma_r^{b,0}$
is chosen to coincide with the the state on the sub-branch with the smallest value of $q_r^{b}$; thus,
\( \Sigma_r^{b,0} = \Sigma_r^a \) for the first sub-branch and \( \Sigma_r^{b,0} \) is taken to be close to \( \Sigma_{doub,r}^M \) for the third sub-branch (see Section 4.2.1 of Part I).

The reference curve (13)–(14) together with the Mie-Grüneisen equation (7) and (16) provide a complete single-phase EOS. Clearly, equation (7) is an adequate approximation for the states \( \Sigma = (v, q, u) \) close to the reference curve. Thus we can only guarantee the validity of the EOS introduced in this section for regimes with \( q > 0 \). (These are the only regimes arising in the experiments and calculations we consider in this paper. Use of other reference curves would be necessary for the expansive branch \( q < 0 \), e.g. a Murnaghan isentropic EOS as in (Miller & Puckett, 1996).)

**Remark 4** It seems more appropriate to approximate the projection of the third sub-branch onto the \((u, s)\)-plane by a parabola in the vicinity of the point \((u_r^{b,0}, s_r^{0})\)

\[
 s = s_r^{0} + s_{r,1} (u_r^{b} - u_r^{b,0}) + \frac{1}{2} s_{r,2} (u_r^{b} - u_r^{b,0})^2 = a_r^0 + b_r^0 u_r^{b} + c_r^0 (u_r^{b})^2
\]  

(17)

rather than by a straight line (11). Then, substitution of equation (17) into (I-16) and elimination of the velocity \( u_r^{b} \) leads, once again, to equations (13)–(14) with a new expression for \( s^2 \):

\[
 s^2 (\eta_r^{a,b}, \Sigma_r^{a}, \Sigma_r^{b,0}) = \frac{(a_r^{0})^2}{\left(1 - b_r^0 \eta_r^{a,b})^2 / 2 - 2a_r^0 c_r^0 (\eta_r^{a,b})^2 \right)} \left[ \frac{1}{2\delta} (1 - \sqrt{1 - 4\delta}) \right]
\]  

(18)

where

\[
 \delta = \left[ \frac{a_r^0 c_r^0 (\eta_r^{a,b})^2}{\left(1 - b_r^0 \eta_r^{a,b})^2 / 2 - 2a_r^0 c_r^0 (\eta_r^{a,b})^2 \right)} \right]^2 .
\]  

(19)

The expression in the brackets in (18) can be significantly simplified when the compression \( \eta_r^{a,b} \) is not too large. Indeed, a Taylor series expansion of the square root gives

\[
 \frac{1}{2\delta} (1 - \sqrt{1 - 4\delta}) = 1 + \delta + 2\delta^2 + \ldots ;
\]  

(20)

thus, when \( \delta \ll 1 \) the entire expression in the brackets in (18) can be very accurately approximated by 1. The use of this simplification turns out to be justified for all the problems
addressed in this paper. Indeed, in case of phase transition in iron, $n_{r}^{a,b}$ never exceeds 0.2 in all the experiments modeled here. For the values of $\epsilon$-iron coefficients $a_{r}^{0}$, $b_{r}^{0}$, and $c_{r}^{0}$ presented in Section 4.1 and for $n_{r}^{a,b} = 0.2$, the necessary inequality holds: $\delta = 0.0056 \ll 1$. In case of graphite-to-diamond phase transition, the reference curve for martensite was constructed from static data under linear elasticity assumption (see Section 4.2) which immediately leads to $c_{r}^{0} = 0$.

The material constants needed for the relations introduced in this section were determined from available experimental data for graphite, diamond, $\alpha$- and $\epsilon$-iron. The values of the constants we utilize are given in Sections 4.1 and 4.2.

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