Molecular dynamic simulation of a homogeneous $\textit{bcc} \rightarrow \textit{hcp}$ transition

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We have performed molecular dynamic simulations of a Marten sitic $\textit{bcc} \rightarrow \textit{hcp}$ transformation in a homogeneous system. The system evolves into three Martensitic variants, sharing a common nearest neighbor vector along a $\textit{bcc} \langle 111 \rangle$ direction, plus an $\textit{fcc}$ region. Nucleation occurs locally, followed by subsequent growth. We monitor the time-dependent scattering $S(q,t)$ during the transformation, and find anomalous, Brillouin zone-dependent scattering similar to that observed experimentally in a number of systems above the transformation temperature. This scattering is shown to be related to the elastic strain associated with the transformation, and is not directly related to the phonon response.

64.70.Kb, 61.72.-y, 63.70.+h, 61.43.Bn

I. INTRODUCTION.

The topic of precursor phenomena in martensitic transformations has been the subject of numerous studies over the past two decades. Martensitic systems undergo first-order transitions which are characterized by a lattice strain (sometimes accompanied by a “shuffling” of the atoms associated with a particular phonon mode).

Experimentally, it has been observed from various diffraction measurements that streaking of the Bragg spots occur in the parent phase close to the transformation, indicating an incipient instability towards the formation of the martensitic phase.

There is also evidence that interesting anomalous dynamical behavior occurs concurrently: the experimentally observed phonon peaks become very broad with enhanced scattering occurring at low frequencies. More puzzling, the intensities and shapes of these peaks exhibit unexpected variations between different Brillouin zones. While most of the experimental data were obtained from alloy systems where the effects of stoichiometry variations may be of importance, similar behavior have also been observed in pure metals.

In this paper, we explore the relationship between anomalous phonon behavior and the phase transformation process through molecular dynamics simulations of Zr as a prototypical system, exhibiting a $\textit{bcc}$ to $\textit{hcp}$ transformation. By monitoring the behavior of the dynamic structure factor of the system, we examine the microscopic origin of the anomalous phonon behavior in these systems. We also study the dynamics of microstructure formation during the transformation. To clarify the problem, we will concentrate on homogeneous systems without defects. The effects of inhomogeneity on the dynamical behavior of the transition will be left to a later study.
Scattering lineshapes in first-order structural phase transformations have been previously studied using various analytic treatments and simulations. Such studies, for both first-order and second-order transformations, have focused on the one-phonon contribution to the scattering, which does not exhibit a Brillouin zone dependence, even in a full anharmonic treatment. Furthermore, most of these studies have focussed on models that do not exhibit a true elastic transformation: in the high temperature phase, the linearized phonon frequencies behave as $\omega^2 \to \omega_0^2 + ck^2$ as $k \to 0$, rather than $\omega \to ck$. Such models are more appropriate for transformations such as $bcc \to \omega$, characterized by a “freezing in” of a phonon mode with a finite frequency (and wavevector), rather than the development of a static amplitude of an elastic degree of freedom that occurs in many Martensitic transformations (including the $bcc \to hcp$ transformation).

Another issue with previous work examining the dynamic response of these systems is that most work examines regions of the product (low temperature) phase embedded in the high temperature matrix. This product phase is hypothesized to be due to either defects, or due to long-lived “heterophase” fluctuations from the parent phase. Such studies are not surprising, as long-lived excitations are necessary to produce “central peaks” in the scattering. However, in first-order transformations, the evidence appears to indicate that there is no clear central peak separate from the phonon peaks (and no long-lived fluctuations into the product phase), especially in systems with little disorder.

In a previous paper, which we shall refer to as paper I, we demonstrated that in a homogeneous system, fluctuations in the high-temperature $bcc$ phase can produce “anomalous” scattering, with significantly different scattering in equivalent Brillouin zones. Neutron scattering reveals different line shapes between different Brillouin zones. Thermal diffuse scattering (energy integrated scattering), observed in both X-ray studies and neutron diffraction experiments, is not featureless, as might be expected from usual arguments concerning multiple phonon scattering, but instead shows characteristics that imply a connection with the incipient Martensitic transition. That such characteristic scattering can occur in the absence of static or long-lived fluctuations into the product phase is somewhat surprising, yet is borne out by experimental work. In paper I, we argued that these are due to fluctuations toward, but not into, the low temperature phase.

More recent molecular dynamics simulations have examined the formation of microstructure during a homogeneous $bcc \to hcp$ transformation, utilizing a simple EAM model for zirconium, as well as the effect of stress on the microstructure. These simulations demonstrate a number of key points concerning the formation of microstructure. Of particular importance relevant to the work presented here, they have demonstrated that $fcc$ regions form at the junction of three $hcp$ variants sharing a common $\langle 11\bar{2}0 \rangle$ direction, rather than forming a triple point between twin boundaries, and that the twin regions contain basal plane stacking faults that maintain the $60^\circ$ orientation between $hcp$ variants. The transformation is interpreted to occur via the Nishiyama-Wassermann mechanism (described in Section III below), rather than the Burgers mechanism.

Here, we present similar simulations, with the goal of examining the dynamics during the $bcc \to hcp$ transition, with a focus on the aspects relevant to the neutron and x-ray scattering experiments. Again, we use molecular dynamics as a tool, to examine the microscopic processes associated with the dynamics. We examine the dynamics in real space, to examine the growth process and the final microstructure. The crystallography of the resulting twinned
structure corresponds to experimental results, and those of Pnsook\textsuperscript{22}–\textsuperscript{24}. With respect to the microstructural development, the most significant difference between the work presented here and that of Ref.\textsuperscript{22} is the choice of simulation cell orientation: unlike their simulations, we do not select out one of the \textit{bcc} directions to be along one of our simulation axes, as that favors \textit{hcp} variants with $\langle 11\bar{2}0 \rangle$ along this direction.

We also examine the time-dependent structure factor $S(Q,t)$, which is the equivalent of time-dependent x-ray scattering during the transition. By doing this, we directly demonstrate that the asymmetry in the scattering between different Brillouin zones is strongest during the transition, and is essentially due to the formation and motion of new Bragg peaks during the transition.

**II. DETAILS OF SIMULATIONS.**

We performed the simulations using the same EAM potential as in the previous paper\textsuperscript{20} and described in detail in Ref.\textsuperscript{27}. This potential has a stable \textit{bcc} phase, with phonons in good agreement with experimental results. The difference between the cohesive energies between the \textit{fcc} and the \textit{hcp} structures is small, compared with \textit{ab initio} results, as is common for these types of potentials. The EAM potentials for Ti and Zr are prone to this problem, due to the lack of directional bonding in these descriptions of these materials. Another important caveat is that this potential does not accurately reproduce the $\omega$-phase properties of Zr or Ti: within this potential, the $\omega$-phase structure is mechanically unstable. As a result, dynamics associated with large-amplitude fluctuations towards this structure (corresponding to the \textit{bcc} $\mathbf{q} = \frac{2}{3}[111]$ longitudinal phonon) are not accurately reproduced. In Zr and Ti (and especially in certain alloys, including ZrNb), the large amplitude fluctuations of this will be anharmonic and possibly strongly non-linear, associated with the corresponding \textit{bcc} $\rightarrow \omega$ transformation. This latter transition, while not studied in this work, is an important topic.\textsuperscript{3–7} The work presented here is essentially a model system, examining the dynamics of the \textit{bcc} $\rightarrow$ \textit{hcp} transformation in the simple case where no competing transformation occurs.

The simulations were performed using two different cubic system sizes: $18 \times 18 \times 18$ conventional \textit{bcc} unit cells (11664 atoms), and $36 \times 36 \times 36$ unit cells (93312 atoms). Except as noted, all results presented will be those of the larger system. No qualitative changes occurred as a result of the change in the system size. Periodic boundary conditions were used in all cases. In order to minimally interfere with the dynamics during the transition, the simulations were performed under constant energy conditions, at an energy corresponding to the average energy for the \textit{bcc} phase at 1500 K. During the \textit{bcc} $\rightarrow$ \textit{hcp} transition, the system lowered its potential energy, as can be seen in fig. 1. With constant energy simulations, this produces a slight increase in temperature. For both the $18 \times 18 \times 18$ system and the $36 \times 36 \times 36$ system, this increase was about 40 K. This is a minor change in temperature, and we do not believe that this affects the dynamics of the transition significantly. We have also used constant volume simulations, with a \textit{bcc} lattice constant of 3.68 Å as in paper I. The transformed structure does not develop any significant macroscopic stress. The simulations were performed for 40,000 time steps, sufficient to observe the transition and subsequent equilibration. This will be demonstrated in the following section.
III. DEVELOPMENT OF MICROSTRUCTURE DURING THE TRANSITION.

We begin with a review of the crystallography of the $bcc \rightarrow hcp$ transition. This is most commonly stated in terms of the Burgers relationship,

$$ (110)_{bcc} \parallel (0001)_{hcp} \quad [1\overline{1}1]_{bcc} \parallel [1\overline{1}20]_{hcp}. $$

The transformation occurs by “shuffling” of alternate (110) planes in the $bcc$ lattice, simultaneous with a shearing of the (112) planes along the [111] direction. (In this paper, we will commonly use three indices for directions and planes in the $bcc$ lattice, and four for directions and planes in the $hcp$ lattice. We will indicate the lattice structure explicitly where we wish to emphasize the lattice correspondence, but otherwise will omit these labels.) The (112) direction then becomes a prism plane in the $hcp$ lattice. With these dynamics in mind, we may rewrite the Burgers relationship as

$$ (\overline{1}1\overline{2})_{bcc} \parallel (\overline{1}100)_{hcp} \quad [\overline{1}1\overline{1}]_{bcc} \parallel [1\overline{1}20]_{hcp}. $$

The shearing of the lattice along $\{1\overline{1}2\}$ planes plays an important role in understanding the anomalous scattering, as will be shown in section 4. Note that if the $[1\overline{1}20]_{hcp}$ direction is along the [111]$_{bcc}$ direction, then there are three different $\{110\}$$_{bcc}$ planes that can become $hcp$ basal planes, namely the (101), (011) and (110) planes. With four equivalent $\langle 111 \rangle_{bcc}$ directions in the $bcc$ lattice, there are 12 $hcp$ variants that may occur. In our simulated microstructure (described below), the system spontaneously selects out one of the $\langle 111 \rangle_{bcc}$ directions, and forms three $hcp$ variants from the associated $\{110\}$$_{bcc}$ planes.

We now establish that there is a transition during our simulations. The most direct approach is to examine the potential energy vs. time during the transition. This is shown in fig. 1, for both the $18 \times 18 \times 18$ and $36 \times 36 \times 36$ system sizes. As can be seen in the figure, both systems spend considerable amounts of time (10,000–20,000 time steps) fluctuating about a value near -6.032 eV. This corresponds to the value obtained at 1500 K for the $bcc$ phase. Both systems then have a rapid drop in the potential energy. This drop continues for some time, then levels off near the value appropriate for the $hcp$ system. Thus, the period during which the potential energy changes systematically serves to approximately identify when the transformational dynamics occur.

Before describing the dynamics of microstructure formation, we present the final microstructure in the system. This is shown for the $36 \times 36 \times 36$ system in fig. 2. Again, results for the smaller system are qualitatively the same. The figure shows the view down the $\{111\}$ direction. There are three different $hcp$ variants present; the $\langle 111 \rangle$ direction forms a $\langle 11\overline{2}0 \rangle$ direction in each of these variants, in accordance with the Burgers relationship.

In the projection shown in fig. 2, the system appears to be very well ordered. Each of the variants forms a “needle-like” domain, extended indefinitely (via the periodic boundary conditions) along the [111] direction. By coloring the atoms according to their potential energy, we have highlighted the twin boundaries between different $hcp$ variants. These boundaries form along $hcp$ (1011) planes, in agreement with experimental observations. As in previous simulations, some of the variants have numerous basal plane stacking faults, allowing for the average angle between $hcp$ domains to be 60°. However, specific twin boundaries deviate noticeably from this value.
We note that in the figure, it is possible to travel from variant II to variant III without passing through such a twin boundary. In fact, there is an fcc region formed where these variants intersect, as indicated in the schematic in the figure. This region is stable throughout the simulation, and is observed in both the $18 \times 18 \times 18$ and $36 \times 36 \times 36$ systems. It is not required to minimize the potential energy of the final configuration: a lower energy configuration would arise from transforming the variant III regions to variant I, and the fcc regions to variant II. This would eliminate the total amount of twin boundary, and would also eliminate the unfavorable fcc region. We note that the $fcc\rightarrow hcp$ energy difference is small in this potential, relative to ab-initio calculations of pure Zr,$^{27}$ suggesting that $fcc$ formation in Zr may be decreased or eliminated in the experimental system. However, some observations of $fcc$ Ti have been made in association with the $bcc\rightarrow hcp$ transformation, as discussed in ref. $^{25}$.

We now examine the time evolution of the system, as it progresses from the $bcc$ to $hcp$ phases. This is shown for the $18 \times 18 \times 18$ system in fig. 3. We focus on the smaller sized system for clarity; the results for the $36 \times 36 \times 36$ system are quite similar. In the figure, we show a slice of the system perpendicular to the [110] direction. The atomic positions have been averaged over 2000 time steps, in order to eliminate the high frequency atomic motions, and reveal the slower dynamics associated with the transformation. The atoms have been colored according to their time-averaged potential energy. Again, this highlights the development of the microstructure.

The first frame of fig. 3 shows the results for time steps 18,000-20,000. Before this, there is little difference between the structure and that of a perfect $bcc$ lattice. This is consistent with fig. 4, which shows the potential energy of the $18 \times 18 \times 18$ system beginning to decrease near step 20,000. In the first frame, the start of the transformation can be seen just left of the center of the system. The vertical rows of atoms show considerable bending around this region, indicating the large accommodation strain required for the nucleus. By the second frame (steps 20,000-22,000) the transforming region is quite clear. In steps 22,000-24,000, the transformed region is starting to develop sharp boundaries, as it extends along the [111] direction. This transformation progresses and the boundaries develop through step 26,000; by steps 26,000-28,000, the transformation is nearly complete, with only the final stages of boundary development remaining. After step 30,000 (not shown), the structure is essentially static.

IV. SIMULATION RESULTS FOR THE STRUCTURE FACTOR.

One of our main objectives is to understand the origin of the pre-martensitic behavior as seen in neutron and x-ray scattering experiments. One of the most notable anomalous behaviors is the difference in thermal diffuse scattering between the so-called “ω” points, with strong scattering located at $Q = \frac{1}{3}(774)$, and significantly less scattering at $Q = \frac{1}{3}(558)$. These correspond to equivalent points in the Brillouin zone, with equivalent magnitudes. Furthermore, in a simple one-phonon picture, the dependence of the scattering on the phonon polarizations are also identical. Therefore, from the one-phonon picture, the scattering at these points should be identical. These modes correspond to the $\frac{2}{3}(111)$ longitudinal phonon, which is the mode that leads to the development of the ω-phase. This connection between
the anisotropy and possible precursors is very suggestive. However, as shown in paper I and elaborated on below, a significant difference between these $Q$ vectors is related to the development of the hcp phase, and the dynamics of the transformation to this phase.

We begin by showing the structure factor $S(Q)$ calculated for a smaller system, $12 \times 12 \times 12$ unit cells, which does not transform. The results for scattering in the (110) plane are shown in fig. [4]. This has been calculated in the same manner as the results in paper I. This figure shows that within our simulations, the anomalous behavior is reproduced, with the scattering near $Q = \frac{1}{3}(774)$ significantly greater than that near $Q = \frac{1}{3}(558)$. In our potential, the $\omega$ phase is higher in potential energy than the bcc phase, and is mechanically unstable. Therefore, the results we show here can not be attributed to $\omega$ phase fluctuations. The anomalous scattering can be seen as a ridge extending from the [222] Bragg peak down to the $\frac{1}{3}[552]$ N-point, where a small peak in the scattering occurs.

We note that in these simulations of the bcc phase, there is no evidence of long-lived fluctuations. The pair correlation function $g(r)$ exhibits clear peaks associated with the bcc phase, but none associated with the hcp phase. However, some short-lived fluctuations toward the hcp phase are observed, and are correlated with anomalous scattering (as described in paper I). This is in accordance with both experiments on the high temperature phases [8–12] and theory [13]. Thus, the anomalous scattering can not be ascribed to previously postulated long-lived fluctuations into the hcp phase.

In order to explore the scattering behavior, we examine here the time-dependent scattering at these “strong” and “weak” $\omega$ points in the Brillouin zone. As paper I demonstrated, the difference in scattering between these two points can not be found within the one-phonon contribution, and the full scattering function must be calculated. Moreover, as there are 12 equivalent wave vectors corresponding to each of these points, we must follow the dynamics of each point.

Figure [5] shows $S(Q, t)$ for $Q = \frac{1}{3}(774)$, for the $18 \times 18 \times 18$ system. As indicated previously, the transformation occurs essentially between steps 20,000 and 30,000. In the figure, we see that for three of the wave vectors, intense scattering occurs during the transformation. The scattering is as large as 20 times that of the other wave vectors, or of the same wave vectors before and after the transformation. For the other nine wave vectors, the scattering shows no distinctive behavior before, during, or after the transformation. Figure [6] shows $S(Q, t)$ for $Q = \frac{1}{3}(558)$. In this case, there is no distinctive behavior during the transformation. For three of the wave vectors, the scattering increases by roughly a factor of five once the transformation is complete.

We can understand these results by examining the full scattering $S(Q)$ in the (110) scattering plane as a function of time. Rather than perform the full calculation, we show the scattering calculated from the time-averaged positions, such as those shown in fig. [3]. We show these calculations in figs. [7] and [8]. Note that these figures contain essentially static information about the microstructure. Before the transformation is initiated (steps 14,000-16,000), the structure factor shows the Bragg peaks expected for the bcc lattice, plus some weak scattering near the N-point phonons at $Q = \frac{3}{2}x\{1\}$ and at $Q = \frac{3}{2}x\{3\}$. Some smearing of the Bragg peaks along the [112] direction is evident. In steps 16,000-18,000, the scattering at the N-points has intensified.

The most dramatic change to the scattering (and the most important to understanding the anomalous scattering) is seen in steps 18,000-20,000. The N-point phonons are now
developing into static Bragg peaks, and the Bragg peaks are now shifted from their bcc lattice positions. The shearing along the [112] direction is evident. This shear brings scattering towards the $\mathbf{Q} = \frac{1}{3}(774)$ scattering vector, while leaving little scattering in the $\mathbf{Q} = \frac{1}{3}(558)$ direction. This is maintained through step 26,000 - essentially, until the transformation is nearly complete. The Bragg peaks now are clearly arranged in a hexagonal pattern. Thus, the anomalous large scattering near $\mathbf{Q} = \frac{1}{3}(774)$ is not from phonon scattering from $\frac{2}{3}[111]$ phonons, but from essentially static displacements associated with N-point phonons combined with shears in the [112] direction. These are exactly the displacements needed for the formation of the hcp phase. From step 26,000 on, the primary development is the narrowing of the peaks along the [111] direction, corresponding to the formation of long, needle-like domains in this direction as seen in the real space pictures in fig. 3. The Bragg peaks also settle into their final positions, with little remnant scattering in the $\mathbf{Q} = \frac{1}{3}(774)$ or the $\mathbf{Q} = \frac{1}{3}(558)$ directions.

We also note that during the course of the transformation, a Bragg peak develops near $\mathbf{Q} = \frac{4}{3}[111]$. This is a result of the differing hcp variants (and the fcc region, as well) developing nearest neighbor lattice vectors along the [111] direction. For real systems (i.e. Ti and Zr) the presence of this developing Bragg peak clouds the issue of interpreting the dynamic behavior of the high temperature phase at this wave vector, as anomalies can be associated either with the $\text{bcc} \rightarrow \text{hcp}$ or the $\text{bcc} \rightarrow \omega$ transformation.

V. DISCUSSION.

The main purpose of this paper has been to explore the dynamics of the $\text{bcc} \rightarrow \text{hcp}$ transformation, and to relate this to the anomalous diffuse scattering observed in the $\text{bcc}$ phase. By examining the time-dependent scattering during the scattering, we have shown that the Brillouin-zone dependence of the scattering is greatest during the transformation, and is due to the formation and shearing of the Bragg peaks as they form the hcp reciprocal lattice. The peaks move through the $\mathbf{Q} = \frac{1}{3}(774)$ region of reciprocal space, creating intense scattering at this wave vector, but their final position is not at this point. There is no such movement through the $\mathbf{Q} = \frac{1}{3}(558)$ point; hence the difference in scattering at these points. A one-phonon picture, taken from the $\text{bcc}$ lattice, would predict identical scattering at these points, even in a fully anharmonic theory. Previous work has relied upon this approximation.$^{13-17}$

We may now clearly explain the anomalous diffuse scattering along the ridge between the $\mathbf{Q} = [222]$ bcc Bragg peak and the N-point $\mathbf{Q} = \frac{1}{3}[552]$ position. This scattering is due to regions of the $\text{bcc}$ lattice fluctuating towards the hcp lattice, with the result that intensity develops at the N-point, and shifts along the $[\bar{1}12]$ direction. These are precisely the modes required to take the $\text{bcc}$ lattice towards the hcp lattice, as in Eq. 2. This interpretation is consistent with previous simulations of the $\text{bcc}$ lattice.$^20$

We have also examined the microstructure development during the transformation. In the beginning of the simulations, there are four equivalent $\langle111\rangle$ directions in the $\text{bcc}$ lattice. (Previous simulations have chosen periodic cells that break the symmetry between these directions.$^21$) The final microstructure corresponds to domains of three different hcp variants, sharing a common $\langle1120\rangle$ direction along one of the original $\langle111\rangle$ directions. These domains are extended along this direction as well (corresponding to “needle-like” domains).
In addition, there is a domain in the metastable fcc lattice. The final domain structure does not minimize the potential energy; a lower energy microstructure with two hcp domains would satisfy the constraints imposed by the cubic simulation cell. Thus, the domain structure must arise out of the dynamics of the transformation process.

The hcp variants are separated by \{10\bar{1}1\} twin boundaries, in accordance with experimental observations. These boundaries lie approximately along the bcc \{112\} planes, as shown in fig. 2. However, in some regions, these boundaries are not flat, caused by basal plane stacking faults within the hcp variants. Pinsook has discussed the formation of these stacking faults in terms of “transformation plasticity”, and argues that these are necessary for the boundaries to lie parallel to the bcc lattice's \{112\} planes, which intersect at 60° degrees, instead of the slightly different angles formed by an ideal \{10\bar{1}1\} hcp twin boundary (55.9° for an ideal c/a ration). However, in our simulations, the boundaries often significantly deviate from being parallel to the bcc \{112\} planes, indicating that more stacking faults occur than would be indicated by these geometric arguments. In both our simulations and those in ref. 22–24, the hcp basal plane stacking fault energy is lower than expected for Zr, which makes comparison with the experimental system difficult.

The dynamics of the transformation correspond to a localized nucleation event, followed by growth of the domains. This is seen quite clearly in fig. 3. Such a picture is inconsistent with recent simulations of a dislocation-nucleated bcc→hcp transformation in which a bcc \(b = \langle 100 \rangle\{011\}\) dislocation nucleates the transition via a long wavelength distortion that evolves into a set of twin boundaries. However, this latter work is dependent on the particular dislocation; similar work with a \(b = 1/2\langle 110 \rangle\{110\}\) dislocation showed different dynamics. This work is also different from that of Pinsook and Ackland, who observed plate-like geometry very quickly from a quenched simulation. In this latter work, the transition is homogeneous; unlike the work presented here, however, one of the \{111\} bcc directions is singled out in the simulation cell. The effect of this on the dynamics is unclear. They also observed an fcc region, but in their simulations, this was a transient phase that was eliminated during the subsequent microstructural evolution. The presence of this region is likely to be sensitive to the choice of interatomic potential; for the work presented here (and, to a lesser extent, the potential used in Refs. 22–24), the difference between the cohesive energies of the fcc and hcp phases is small compared to the actual value in Ti and Zr, making the appearance here more likely.

The present work provides a clear demonstration of the relationship between the dynamics of the bcc→hcp transformation, and the anomalous scattering observed in the parent phase. The observed zone-dependence does not require defects or static transformed (or distorted) regions in the lattice; this is clear from the simulations presented here and previously, and from experimental studies of pure metals. This is an important step in understanding the experimental results on the pre-transition dynamics, as measured through scattering experiments. Further work is required to understand how these dynamics are affected by defects, compositional fluctuations in alloy systems, and the competing bcc → \(\omega\) transformation.
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FIG. 1. Potential energy versus time step, for the $18 \times 18 \times 18$ and $36 \times 36 \times 36$ system sizes. The large change in the potential energies is due to the $bcc \rightarrow hcp$ transition.

FIG. 2. Final microstructure of $36 \times 36 \times 36$ system, as viewed down the $[1\bar{1}\bar{1}]$ direction, in a completely relaxed (zero force) configuration. The different atomic shadings indicate the potential energy of the atoms, with large, dark atoms having the highest energy; large, gray atoms having the lowest energy; and the smaller, lightest atoms having intermediate energies. This highlights the twin boundaries between $hcp$ variants. There are three such variants in the final microstructure, extending along the $[1\bar{1}\bar{1}]$ direction, plus an $fcc$ region as indicated in the schematic picture shown in the lower right part of the figure.

FIG. 3. Time-averaged positions of atoms during the steps indicated. The colors indicate the time-averaged potential energy, with blue being the lowest and red the highest.

FIG. 4. The static structure factor $S(Q)$ calculated from simulations of the $bcc$ phase, as shown in the $(1\bar{1}0)$ scattering plane. The x-axis corresponds to the $[1\bar{1}0]$ direction; the y-axis corresponds to the $[001]$ direction.

FIG. 5. Time-dependent scattering at the 12 different $Q = \frac{1}{3}(774)$ wave vectors. As can be seen, those wave vectors whose directions are closest to $[111]$ exhibit large scattering during the transformation. Note the differences in scales between graphs.

FIG. 6. Time-dependent scattering at the 12 different $Q = \frac{1}{3}(558)$ wave vectors. Unlike the scattering at the $Q = \frac{1}{3}(774)$ wave vectors, there is little change in scattering during the transformation.

FIG. 7. $S(Q)$ calculated from the time-averaged structures (as shown in fig. 3) for different time steps. The scattering plane is the same as in fig. 4.

FIG. 8. $S(Q)$ calculated from the time-averaged structures (as shown in fig. 3) for different time steps. The scattering plane is the same as in fig. 4.
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