DISORDER-DRIVEN NONEQUILIBRIUM MELTING STUDIED BY ELECTRON DIFFRACTION, BRILLOUIN SCATTERING, AND MOLECULAR DYNAMICS*

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Disorder-Driven Nonequilibrium Melting Studied by Electron Diffraction, Brillouin Scattering, and Molecular Dynamics

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ABSTRACT

In the present paper, a brief overview of our electron diffraction, Brillouin scattering and molecular dynamics studies of radiation-induced amorphization of ordered intermetallic compounds is presented. In these studies, measured changes in the velocity of surface acoustic phonons, lattice constant, and the Bragg-Williams long-range order parameter induced by irradiation were compared with the results of computer simulations of defect-induced amorphization. The results indicate that progressive chemical disordering of the superlattice structure during irradiation is accompanied by an expansion of the lattice and a large change in sound velocity corresponding to a ~50% decrease in the average shear modulus. The onset of amorphization occurs when the average shear modulus of the crystalline compound becomes equal to that of the amorphous phase. This elastic softening criterion for the onset of amorphization and the dependence of the average shear modulus on the long-range-order parameter are in excellent agreement with molecular dynamics simulations. Both the experimental observations and computer simulations confirm the predictions of the generalized Lindemann melting criterion which stipulates that thermodynamic melting of a defective crystal occurs when the sum of the dynamic and static mean-square atomic displacements reaches a critical value identical to that for melting of the defect-free crystal. In this broader view of melting, the crystal-to-glass transformation is a disorder-driven nonequilibrium melting process occurring at temperatures below the Kauzmann isentropic glass-transition temperature.
1. Introduction

The transformation of a crystalline structure directly to a glassy amorphous state can be induced by a variety of isothermal damage-accumulation processes ranging from energetic particle irradiation, multilayer interdiffusion reactions, hydrogen charging, mechanical alloying, to the application of high pressures and tensile stresses [1,2]. Intriguing parallels between the crystalline-to-amorphous (C-A) transformation and ordinary melting have stimulated considerable interest in the physics of the transformation and its relationship to melting. For example, well-equilibrated metallic glasses have static structure factors very similar to that of a supercooled liquid and, hence, structurally can be regarded as a frozen liquid. And like the liquid phase during melting, the amorphous phase induced by externally-driven disordering processes often nucleates preferentially at defect sinks such as free surfaces, grain boundaries, and dislocations [3]. On the theoretical side, current theories of C-A transformations [4-6], like those for melting [7-10], invoke lattice defects as the fundamental cause of the destruction of the crystalline structure. The primary difference is that heat-induced melting involves thermally-generated defects whereas, for disorder-driven C-A transformations, athermal processes produce the defects. These parallels suggest that the C-A transformation can also be regarded as a melting transformation, albeit a nonequilibrium one occurring at very low temperatures where defect structures are effectively frozen.

In the present paper, a short overview is given of a number of critical studies that contributed to our current understanding of the relationship between the C-A transition and the melting process. The two particle-scattering techniques, Brillouin scattering spectrometry and transmission electron microscopy (TEM), have been very useful in these studies and were first utilized in combination to systematically investigate the effects of radiation damage on amorphization of the intermetallic compound Zr$_3$Al [11]. The results showed that a shear softening similar in magnitude to that which precedes the onset of heat-induced melting also precedes the onset of defect-induced amorphization. On the theoretical side, we have used molecular dynamics (MD) to simulate the effects of radiation-produced defects on the elastic constants of model intermetallic compounds [12-15], and found that the simulated defect-induced shear softening is in good agreement with the Brillouin scattering measurements. Moreover, we show that the onset of defect-induced amorphization is governed by a shear softening criterion for melting which is physically equivalent to a thermodynamic criterion for melting expressed in terms of a generalized version of the melting criterion proposed 90 years ago by Lindemann [16].

2. Experimental Studies

2.1. Techniques
Brillouin scattering and TEM techniques were employed to measure the effects of irradiation dose on the elastic properties, the Bragg-Williams long-range order parameter and lattice expansion of polycrystalline Zr₃Al (L₁₂ superlattice structure). Two types of irradiation were performed. For Brillouin scattering measurements, individual 3 mm-diameter spots on an optically-flat bulk specimen were irradiated with 1-MeV Kr⁺ ions up to various doses, up to 6x10¹⁴ ions/cm². All irradiations were carried out at room temperature in a high-vacuum chamber using a tandem ion accelerator. TRIM [17] calculations, assuming a threshold energy of 25 eV, were used to convert ion dose to average number of displacements per atom (1 dpa = 3.19 x10¹³ ions/cm²) in the first 300 nm, the depth probed by the Brillouin technique. After irradiation, Brillouin scattering spectroscopy was carried out to measure the velocity of the surface wave in each of the irradiated spots and several unirradiated areas. These measurements employed a single-mode Ar laser, polarized in the scattering plane, at 150 mW of power and a wavelength of 514.5 nm. All measurements were made in a backscattering geometry with the incident and scattered beams at 60 degrees from the normal to the specimen surface. The scattered light was frequency-analyzed with a scanning 5+2 Fabry-Perot interferometer. Measured frequency shifts were then used to calculate the surface wave velocity, \( V_S \), given by the formula [18]

\[
V_S = \pm \frac{\lambda \Delta f}{2 \sin \theta} \, ,
\]

where \( \lambda \) is the wavelength of the light, \( \Delta f \) is the frequency shift, and \( \theta \) is the angle of incidence and reflection. The determination of elastic properties from Brillouin spectra requires understanding of how the velocity of surface elastic waves relates to the structure and properties of the surface layers of the material. However, for many purposes, it suffices to note that, for homogeneous, elastically-isotropic media (e.g., metallic glasses or small-grained polycrystalline materials), the surface wave velocity is related to the average shear modulus, \( G = (C_{44} + C')/2 \), by [19]

\[
V_S = \beta(G/p)^{1/2} \, ,
\]

where \( p \) is the density and \( \beta \) is a weakly sensitive function of Poisson’s ratio and usually varies only between 0.3 and 0.4. Hence, changes in the velocity or frequency shift can be used to determine the change in the shear modulus. For example, for a constant density, a decrease of 20% in the velocity or frequency shift measured in the Brillouin spectrometer would indicate a 40% reduction in the shear modulus.
Additional irradiations with 1-MeV Kr\textsuperscript+ ions were carried out inside a high-voltage electron microscope (HVEM) at the Argonne National Laboratory HVEM-Tandem accelerator facility. The in situ HVEM irradiations permitted real-time direct observations of the amorphization process and to obtain electron diffraction patterns required for the determination of the Bragg-Williams long-range order, \( \eta \), and the lattice expansion, \( \Delta a/a_0 \). The in situ irradiations were periodically interrupted, during which two types of diffraction patterns were recorded. Low-index, many-beam, zone-axis patterns were taken to monitor the diffuse intensity halos associated with the formation of the amorphous phase. However, diffraction patterns for \( \eta \) measurements were recorded under weak-beam diffracting conditions with the [400] fundamental reflection strongly excited. The weak-beam diffraction patterns were recorded under constant exposure conditions and processed using standardized photographic developing procedures. After digitizing the negatives with an Optronics scanning microdensitometer, the optical densities (peak height minus background) of the [100] superlattice reflection (IS) and the [200] fundamental reflection (IF) were converted to electron exposure using experimentally determined calibration curves to convert optical density to electron dose. The corrected intensities were subsequently employed to calculate normalized long-range order parameter, \( \eta/\eta_0 \) using the relationship

\[
\frac{\eta}{\eta_0} = \left( \frac{I_S}{I_F} \right)^{1/2} \left( \frac{I_S^0}{I_F^0} \right)
\]

where \( I_S^0 \) and \( I_F^0 \) are the corrected intensities of the fully-ordered, unirradiated sample. The same set of weak-beam diffraction patterns was also used to measure changes in the lattice parameter from the spacing of the [400] strongly-excited beam.

2.2. Experimental Results

Irradiation-induced changes in the electron diffraction effects associated with the C-A transformation in Zr\textsubscript{x}Al are shown in Fig. 1 along with the surface wave velocity, \( V_S \), measured by Brillouin scattering. The selected area diffraction patterns labelled 'a' through 'f' correspond to the ion doses denoted by arrows on the plot of \( V_S \) versus ion dose. The appearance of the a diffuse intensity halo passing through the [111] Bragg spots in diffraction pattern c at an ion dose of 5x10\textsuperscript{13} ions/cm\textsuperscript{2} (= 0.15 dpa) was taken as the evidence for the onset of amorphization. However, the presence of a much weaker and broader diffuse intensity halo in diffraction pattern b, though barely visible, indicates that amorphization had already started earlier by a dose of 3x10\textsuperscript{13} ions/cm\textsuperscript{2}
This combined electron diffraction and Brillouin scattering study was particularly revealing as it shows that all of the shear softening induced by the irradiation occurs prior to the onset of amorphization. Hence, the shear softening is a pre-amorphization effect and not a consequence of amorphization.

Figure 2 shows the Bragg-Williams long-range order parameter $\eta$ (normalized to that of the unirradiated sample), the lattice expansion, $\Delta a/a$, and the quantity, $(V_s/V_o)^2$, where $V_o$ is the surface wave velocity of the unirradiated sample, all plotted as a function of dose expressed in units of displacements per atom (dpa). Note that the dose scale for Fig. 2c is different from those of Figs. 2a and 2b, and that there is a change in dose scale at 0.3 dpa in Fig. 2c. Because the change in density associated with the C-A transformation, as evidenced by the change in lattice parameter, is only about 2%, it follows from Eq. (2) that $(V_s/V_o)^2 = G_s/G_o$, where $G_s$ and $G_o$ are the shear moduli of the irradiated and unirradiated samples, respectively. Hence, the ratio $(V_s/V_o)^2$ provides a direct measure of the shear softening induced by the irradiation. It is clear from Fig. 2 that the softening of the crystalline shear modulus is associated with a progressive destruction of the superlattice structure and that the chemical disordering induces a small expansion of the crystalline lattice of about 0.7%.

The volume dependence of the average shear modulus of irradiated Zr$_3$Al, shown in Fig. 3, is identical in form to that for heating. Both exhibit a linear dependence on volume expansion, as can be seen by comparing Fig. 3 with Fig. 4 which shows the shear elastic constants ($C'$ or $C_{44}$) of a number of simple metals as a function of the thermal volume expansion during heating to melting [20]. The vertical dashed line in Fig. 3 denotes the disorder-induced expansion at the onset of amorphization and those in Fig. 4 denote the specific volumes of the metals at the their thermodynamic melting temperature $T_m$. The similarities are striking. Although the critical volume expansion for thermodynamic melting is about twice that for the onset of amorphization, the magnitude of the shear softening at which melting or amorphization begins is about the same for the two processes, i.e. about 50%.

Figure 2c reveals another interesting correlation. It shows that the onset of amorphization occurs at a dose of about 0.1 dpa where the decreasing surface wave velocity of the damaged crystal first becomes equal to the surface wave velocity in the fully amorphous phase. This correlation suggests that the free energy of the damaged crystal becomes equal to that of the amorphous phase when the shear moduli of the two phases become equal. This elastic softening criterion for the onset of amorphization can be seen more clearly in Fig. 5, where $(V_s/V_o)^2$ is plotted as a function of the mean-square chemical disorder defined by $(1 - \eta^2)$. As shown theoretically by Krivoglaz [21] and experimentally by Burbank et al. [22], the quantity $(1 - \eta^2)$ is proportional to $\langle \mu^2 \rangle$ in partially-
ordered A3B alloys having the L12 (Zr3Al) or A15 (Nb3Sn) type superlattice structures. Hence, as will be shown in Section 4, the linear dependence of \((V_s/V_o)^2 = G_d/G_o\) on \((1 - \eta^2)\) in Fig. 5 provides a direct confirmation of the generalized Lindemann melting criterion [1]. The horizontal dashed line in Fig. 5 represents the value of the shear modulus for the completely amorphous Zr3Al alloy, and the arrow denotes the value of the mean-square chemical disorder of 0.85 \((\eta = 0.38)\), corresponding to the onset dose for amorphization of ~0.1 dpa. Figure 5 reveals two important features. First, it shows that the average shear modulus is a linearly-decreasing function of \((1 - \eta^2)\); and second, that the onset of amorphization occurs very close to a critical value of the mean-square chemical disorder \((1 - \eta^2)\), where the shear modulus of the damaged crystal \(G_d\) first becomes equal to that of the fully amorphous state, \(G_a\). As will be shown in the following sections, this elastic softening criterion has been confirmed by molecular dynamics simulations, and is predicted by a simple analytical model for amorphization that is based on a generalized version of the Lindemann melting hypothesis.

3. Molecular Dynamics Simulations

Molecular dynamics simulations, using embedded atom potentials fitted to the thermodynamic properties, lattice constants and elastic properties of several intermetallic compounds, were performed to study the effects of antisite defects and Frenkel pairs in destabilizing the crystalline lattices at constant temperature \((T = 30 \text{ K})\) and pressure \((P = 0)\) [see [12-15] and references therein]. Figure 6, for example, shows the computer-simulated structural evolution of the compound NiZr2 during antisite defect creation, as revealed by the changes in [001] atomic projections, and the corresponding many-beam electron diffraction patterns calculated by the multislice method of Cowley and Moodie [23,24]. Also shown are the potential energy, \(\Delta E/N\), volume expansion, \(\Delta V/V_o\), the shear elastic constants, \(C_{44}\) and \(C' = (C_{11} - C_{12})/2\), and the average shear modulus, \(G_d\), plotted as a function of dose expressed as exchanges per atom (epa). An epa of unity means that, on average, the atomic positions of every Ni-Zr atom pair have been exchanged once. The effects of Frenkel pairs on the same quantities were also investigated as a function of dose expressed as displacements per atom (dpa). For both types of defects, the intensity of superlattice reflections weakens with dose indicating a gradual loss of long-range order. Weak intensity halos associated with the onset of amorphization first appear on the calculated diffraction patterns at about 0.13 epa for antisite defects and about 0.16 dpa for Frenkel pairs.

The MD results in Fig. 7 show the dose dependence (in units of epa) of the Bragg-Williams long-range order parameter \(\eta\) and the normalized average shear modulus \(G_d/G_o\). The qualitative feature of the calculated dose dependence is strikingly similar to that of the measured
dose dependence of $\eta$ and $(V_s/V_o)^2$ shown in Fig. 2. Moreover, the results in Fig. 8 show that the square of the calculated Debye temperature, $\theta_d^2$, which scales linearly with $(V_s/V_o)^2$, is a linearly decreasing function of the mean-square chemical disorder $(1 - \eta^2)$, in agreement with the experimentally observed changes in $(V_s/V_o)^2$ illustrated in Fig. 5. In further agreement with experiment, the onset of amorphization, as evidenced by the first clear appearance of an intensity halo in the computed electron diffraction patterns, occurs at a value of the mean-square chemical disorder where $\theta_d^2$ becomes equal to that of the amorphous phase. This correlation confirms once again that the onset of amorphization is governed by the shear-softening criterion, $G_d = G_o$.

4. Discussion

Okamoto et al. [1] showed that the shear softening criterion $G_d = G_o$ for amorphization follows from the generalized Lindemann melting hypothesis and the fact that the free energy of the damaged crystal becomes equal to that of the fully relaxed glass when the polymorphous melting temperature of the damaged crystal, $T_m^d$, becomes equal to the glass transition temperature, $T_K$, of the fully relaxed glass of the same composition. The generalized Lindemann melting hypothesis can be expressed in the form of a scaling relationship between the reduced quantities $T_m^d/T_m^o$, $\theta_d^2/\theta_o^2$, and $G_d/G_o$ and damage level, measured by the mean-square static displacement $\langle \mu_{st}^2 \rangle$ [1], i.e.,

$$\frac{T_m^d}{T_m^o} = \frac{\theta_d^2}{\theta_o^2} = G_d = G_o = \left[ 1 - \frac{\langle \mu_{st}^2 \rangle}{\langle \mu_{cn}^2 \rangle} \right]$$

(4)

where $T_m^o$, $\theta_o$, and $G_o$ are the melting temperature, Debye temperature, and average shear modulus of the perfect crystal, respectively, and $\langle \mu_{cn}^2 \rangle$ is a constant equal to the mean-square thermal displacement at the thermodynamic melting temperature of the defect-free crystal. It follows from Eq. (4) that the elastic softening criterion $G_d = G_o$ is equivalent to the thermodynamic criterion for amorphization $T_m^d = T_K$. Hence, the condition $G_d = G_o$ can be called the Lindemann thermodynamic criterion for amorphization because it depends on the validity of the generalized Lindemann hypothesis expressed in the form of Eq. (4).

The disorder-induced softening of the average shear modulus described by Eq. (4) is identical in form to the isobaric, heat-induced softening as seen, for example, in Fig. 9, which shows
the temperature dependence of $C_{44}$ and $C'$ for Al [25]. Also shown is the average shear modulus $G$. That the form of the shear softening is indeed identical for the two processes follows from the general form of the temperature dependence of the isobaric elastic constant of many metals [26]

$$\frac{G_o(T)}{G_o(0)} = \exp(-T/T_{cri}) . \tag{5}$$

Here, $G_o(0)$ is the average shear modulus at $T = 0$ K, and $T_{cri}$ is the temperature at which $G_o(T)$ extrapolates to zero on the temperature axis. Typically, $T_{cri} >> T_m^0$, so that for $T \leq T_m^0$, Eq. (5) reduces to the linear form $G_o(T)/G_o(0) = [1 - T/T_{cri}]$. This linear form is identical to Eq. (4) because $T/T_{cri} \approx \mu_{vib}^2/\mu_{sta}^2$. Consequently, if the generalized Lindemann melting hypothesis described by Eq. (4) is correct, then the same curve should be obtained for both isothermal disordering and isobaric heating when $G_d$ is plotted as a function of the total mean-square atomic displacement, $\langle \mu_{tot}^2 \rangle = \langle \mu_{vib}^2 \rangle + \langle \mu_{sta}^2 \rangle$. Moreover, the resulting curve should be independent of the defect structure, because the generalized Lindemann melting criterion depends only on the magnitude of $\langle \mu_{sta}^2 \rangle$ and not on its physical origin. This prediction was confirmed by molecular dynamics simulations of heat-induced melting and defect-induced amorphization of the compounds FeTi, NiZr, and NiZrz [12-15]. Furthermore, Debye-Waller factors for boron-implanted Ni alloys determined from energy-filtered electron diffraction measurements [27] have shown that the critical value of the Lindemann parameter is, within experimental error, identical to that for thermodynamic melting of Ni, i.e., $\delta_{cri} = 0.12$. The latter value was obtained by linearly extrapolating lower-temperature (100 – 900 K) measurements of $\langle \mu_{vib}^2 \rangle^{1/2}$ [28,29] and the nearest-neighbor distance, $d_{nn}$, reported in the literature for Ni [30] to $T = 1728$ K, the thermodynamic melting temperature of Ni.

5. Conclusion

We used a combination of particle-scattering techniques - electron diffraction and Brillouin scattering spectrometry - and MD simulations to study the kinetics of radiation-induced C-A transitions in intermetallic compounds. The experimental and MD results both show that the onset of defect-induced amorphization of ordered compounds occurs when $G_d = G_K$, where $G_d$ and $G_K$ are the average shear modulus of the crystalline and amorphous phases, respectively. This shear softening criterion for the onset of amorphization is consistent with the Lindemann thermodynamic
criterion for amorphization, for which the condition $G_d = G_k$ corresponds to a critical degree of static atomic disorder where the free energy of the damaged crystal becomes equal to that of the amorphous phase. This generalized Lindemann melting hypothesis assumes that melting of a defective crystal occurs when the total root-mean-square atomic displacement, i.e., the sum of its static and thermal components, reaches a critical fraction of the nearest-neighbor distance which is identical to that for thermodynamic melting of the defect-free crystal. Because the melting criterion depends only on the magnitude of the total mean-square atomic displacement but not on how the displacements are produced, it should be independent of the specific nature of the defect structure. Furthermore, within the framework of the generalized Lindemann melting criterion, an increase in the static atomic displacements at constant temperature has the same effect on the shear modulus and, hence, on the melting temperature of the crystalline phase as an increase in temperature at constant pressure. Therefore, the generalized Lindemann melting criterion should be universal, applicable not only to heat-induced melting, but also to a broad spectrum of isothermal damage-accumulation processes. This prediction has been confirmed by recent experiments that show that, within experimental error, the critical value of the generalized Lindemann parameter for the onset of amorphization of Ni during implantation with boron ions at 77 K is identical to that for thermodynamic melting of Ni.

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References

Figure Captions

Figure 1. Changes in the [112] zone-axis electron diffraction patterns and the velocity of surface waves in Zr₃Al as a function of ion fluence during irradiation with 1-MeV Kr⁺ ions at room temperature.

Figure 2. Changes in the Bragg-Williams long-range order parameter, volume expansion, and surface wave velocity as a function of displacement dose for 1-MeV Kr⁺-bombarded Zr₃Al.

Figure 3. Volume dependence of the average shear modulus (Gₐ/Gₒ) during Kr⁺ irradiation of Zr₃Al. The dashed vertical line indicates the volume expansion for the onset of amorphization.

Figure 4. Volume dependence of the shear elastic constants (C₄₄ or C') associated with heating to melting of various simple metals. The dashed vertical lines denote the volume expansions of the metals at their thermodynamic melting temperatures.

Figure 5. Relative change in the surface wave velocity squared as a function of the mean-square chemical disorder. The horizontal dashed line represents the value of this quantity in the fully amorphous state, and the vertical line indicates the onset of amorphization.

Figure 6. Results of molecular dynamics simulations showing the effects of chemical disorder on the phase stability of NiZr₂ as revealed by the [001] atomic projections and their corresponding computer-calculated electron diffraction patterns. Also shown are the potential energy per atom (ΔE/N), the volume expansion (ΔV/V₀), and the shear elastic constants (C₄₄, C', and Gₐ) as a function of dose expressed in units of exchanges per atom (epa). The arrows denote the doses corresponding to the depicted atomic projections and their diffraction patterns.

Figure 7. Computed changes in the Bragg-Williams long-range order parameter and the normalized average shear modulus of NiZr₂ as a function of dose in epa.
Figure 8. Computed changes in the square of the Debye temperature as a function of the mean-square chemical disorder \((1 - \eta^2)\) in NiZr₂.

Figure 9. Temperature dependence of the shear elastic constants \(C_{44}\) and \(C' = (C_{11} - C_{12})/2\) for Al. Also shown is the average shear modulus \(G = (C_{44} + C')/2\). The vertical dashed line denotes the thermodynamic melting temperature of Al.
2.8

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i

i

2.6

●

2.4

●

~

3 MeV Kr → Zr₃Al

1.8 — 320 K

1.6

1.4

1.2

1.0

10¹¹

10¹²

10¹³

10¹⁴

10¹⁵

DOSE (ions/cm²)

DOS (ions/cm²)

1 MeV Kr → Zr₃Al

320 K

Vₙ (10⁵ cm/s)

Fig. 1
Fig. 2
1-MeV Kr $\rightarrow$ Zr$_3$Al

$G_d/G_o$

$3\Delta a/a_o$ (%)  Instability

Fig. 3
Fig. 4

Shear modulus (10^{10} \text{ Pa})

\Delta V/V_o

- Zn
- Al
- Cd
- Pb

● solid
○ melt
Onset of C→A

1-MeV Kr⁺ → Zr₃Al

Amorphous Zr₃Al

\( (V_s/V_s^0)^2 \)

\( 1 - \eta^2 \)

Fig. 5
Fig. 6
Fig. 7

- Onset of amorphization
Fig. 8
Fig. 9

Elastic Moduli ($10^{10}$ Pa)

Temperature (K)