Elastic instability of crystals caused by static atom displacement: A mechanism for solid-state amorphization

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During the solid-state amorphization process, there have been a number of observations showing a large lattice dilatation and softening of shear elastic constants. Based on these reports, the amorphization mechanism was modeled by introducing static displacement of atoms that caused lattice strain. The calculation indicated that a crystalline structure became unstable at a critical strain value. Qualitative agreement was obtained between the calculated and experimental values of the changes in the shear elastic constant and the lattice parameter at the instability point.

I. INTRODUCTION

Crystal-to-amorphous transformation (amorphization) can take place in a wide range of materials by means of various solid-state techniques.[1] These techniques include high-energy particle irradiation, ion implantation, hydrogen charging, ion-beam mixing, annealing of diffusion couples, mechanical alloying, and mechanical deformation. A basic premise of amorphization is to increase the free energy of the original crystalline phase to a point higher than that of an amorphous phase without transforming to other crystalline phases. The free energy can be raised either by forming a nonequilibrium solid solution[1] or by accumulating lattice defects such as antisite defects,[2] Frenkel pairs,[3] point defect clusters,[4] and dislocations.[5] Transformation to other crystalline phases can be kinetically restricted by performing the amorphization process at a relatively low temperature.[6]

Despite the variety of amorphization techniques, there appears to be a common observation; lattice strain and the softening of shear elastic constants occur before the onset of amorphization. The necessity of the elastic softening to amorphization is clearly demonstrated in Table I for intermetallic compounds irradiated with high-energy Kr ions.[7-10] Shear elastic constants of the compounds that were amorphized exhibited more than 40% decrease. On the other hand, shear elastic constants of NiAl and FeAl that did not undergo amorphization exhibited only 10–20 % decrease. Table I also lists the reported values of lattice parameter variation during irradiation. In contrast to the shear elastic constant, it appears at the first sight that the change in the lattice parameter does not have any relationship with the amorphization tendency. However, the following evidences suggest the importance of the lattice strain to amorphization. During Kr-ion irradiation of Zr_3Al,[8] a 0.8% increase in the lattice parameter was observed before the onset of amorphization, as shown in the Table. When the same material was amorphized by hydrogenation,[11] the lattice parameter was found to increase by the same magnitude prior to amorphization. Although the shear elastic constant was not reported for a hydrogenated Zr_3Al, the Gruneisen relationship[12] requires that the same decrease (50%) in the shear elastic constant be observed for the same dilatation value.

Similar results have been reported in thin films of Si. As the grain size of hydrogenated polycrystalline silicon was decreased by controlling the deposition conditions, abrupt transformation from a crystalline phase to an amorphous phase was observed at a grain size of ~ 30 Å. The lattice parameter of the specimen near the transition point was found to be $\sim 1\%$ greater than that of a much larger grain specimen.[13] Coincidentally, when Si was amorphized by self-ion implantation,[14] the same magnitude of lattice strain was observed before amorphization took place, as identified by an x-ray rocking curve technique. Consistent results were obtained by analyzing a shift of a crystalline Raman peak.[15] Since the peak shift was larger than the calculated value using a reported force constant and a lattice parameter change of 1% in Si, reduction of the force constant was suggested to accompany the observed strain. These results suggest that amorphization occurs when the crystal is strained to a critical value that is dependent on materials. The critical magnitude of strain appears to result in a large decrease (40–50 %) in the shear elastic constant that is independent of materials.

TABLE I. Reported amorphization tendency $(C \rightarrow a)$ by ion irradiation, lattice parameter increase $(\Delta a / a_0)$, and shear elastic constant decrease $(-\Delta C / C_0)$ for various intermetallic compounds.

	$C \rightarrow A$	$\Delta a / a_0$ (%)	$-\Delta C / C_0$ (%)
Nb_3Ir			52[a]
Zr_3Al	Yes	0.8	50[b]
CuTi			40[c]
FeTi		1.3~2.0	40[d]
FeAl	No		20[c]
NiAl		0.67	10[d]

[a]Reference 7.
[b]Reference 8.
[c]Reference 9.
[d]Reference 10.

The following evidence in other materials amorphized by different methods further supports the importance of the elastic softening and lattice strain to amorphization. During B-ion implantation into Nb,[16] the mean-square displacement amplitude of atoms, determined by the x-ray diffuse scattering intensity, was found to increase rapidly and saturate at the onset of amorphization. Such atomic displacement would lead to the softening of the shear elastic constant due to the elastic anharmonicity. Amorphization has also been reported in the NiTi intermetallic compound by cold working.[5] Estimated lattice dilatation and associated decrease in the shear elastic constant caused by dislocation accumulation were found to be comparable in magnitude to those in Table I.[17]

Consistent results have been reported theoretically by molecular-dynamics simulation of the amorphization process. The radial distribution function, coordination number, and mean-square displacement amplitude of lattice atoms were calculated as interstitials were inserted into an fcc structure followed by structural relaxation.[18] It was found that with increasing the interstitial concentration, the mean-square displacement increased and the radial distribution function and coordination number approached those of an amorphous structure. Similar results were obtained in $NiZr_2$ during introduction of antisite defects[19] and NiZr during introduction of either Frenkel pairs or antisite defects.[20] In NiZr, the accumulation of Frenkel pairs or antisite defects were both found to increase the crystalline volume by 4% and decrease the shear elastic constant by ~50% before the onset of amorphization. It has been also shown[21] that a large decrease of the shear elastic constant occurs during introduction of antisite defects in materials that fit with the empirical criteria for amorphization,[22] indicating a close link between the amortization mechanism and the softening of the shear elastic constant.

These experimental and theoretical results have all indicated directly or indirectly that during the course of amorphization, lattice atoms are displaced from their equilibrium lattice sites, causing lattice strain and the softening of shear elastic constants to critical values. In this regard, the amorphization mechanism has often been paralleled with the melting phenomena[1,8] described by the Gibbs' criterion of the crystalline instability caused by lattice dilatation and the decrease of the elastic constants to a null value.[23] We are unaware of an attempt to describe explicitly the effects of lattice dilatation and softening on the crystalline stability. This work is intended to describe the amorphization mechanism in terms of the elastic instability caused by static displacement of atoms. The variation of the interatomic distance was calculated as a function of the defect concentration. An instability point of the crystalline structure was found to exist where the lattice strain diverges to infinity. Qualitative agreement was found between the calculated values and the experimental values of the shear elastic constant and the lattice parameter increase at the instability point.

II. THEORY

The present theory for amorphization is derived from the melting theory developed by Ida,[24] based on the elas-

tic anharmonicity accompanied by the vibrational elongation of interatomic spacings that increased with increasing temperature. In the case of solid-state amorphization that occurs at a low temperature, thermal vibration is not a major cause for the elongation of interatomic spacings and is thus neglected in the present work. Instead, static displacement of atoms from their lattice site is a dominating phenomenon as a manifestation of lattice defects introduced during the amorphization process.

Let us suppose for simplicity that the crystal in consideration consists of a single element and is elastically isotropic. Static displacement of the nth atom can be described by the following Fourier series:

$$\mathbf{u}_n = \sum_{\mathbf{k}i} \alpha_{\mathbf{k}i} \cos(\mathbf{k} \cdot \mathbf{a}_n) \mathbf{q}_{\mathbf{k}i} . \tag{1}$$

Here, $\alpha_{\mathbf{k}i}$ is a displacement amplitude, $\mathbf{k}$ is a wave vector, i represents each normal mode of vibration ($i = 1$ for the longitudinal mode and $i = 2, 3$ for the two independent transverse modes), $\mathbf{a}_n$ is a position vector of the nth atom, and $\mathbf{q}_{\mathbf{k}i}$ is a polarization vector of corresponding vibration modes.

When we define a new position vector, $\mathbf{r}_n = \mathbf{a}_n + \mathbf{u}_n$, after static displacement of $\mathbf{u}_n$, the fractional increase of the interatomic distance (i.e., strain) between the nth and n'th atoms can be given as

$$Q = \frac{|\mathbf{r}_{n'} - \mathbf{r}_n| - |\mathbf{a}_{n'} - \mathbf{a}_n|}{|\mathbf{a}_{n'} - \mathbf{a}_n|} . \tag{2}$$

Expanding $|\mathbf{r}_{n'} - \mathbf{r}_n|$ with respect to $\mathbf{u}_{n'} - \mathbf{u}_n$ up to the second-order term, Q becomes

$$Q = \frac{\mathbf{a} \cdot \mathbf{u}}{a^2} + \frac{1}{2} \left[\frac{u^2}{a^2} - \frac{(\mathbf{a} \cdot \mathbf{u})^2}{a^4} \right] , \tag{3}$$

where $\mathbf{a} = \mathbf{a}_{n'} - \mathbf{a}_n$, $\mathbf{u} = \mathbf{u}_{n'} - \mathbf{u}_n$, $a = |\mathbf{a}|$, and $u = |\mathbf{u}|$. When the scalar product $\mathbf{a} \cdot \mathbf{u}$ is taken for all possible vectors, it is obvious that the first term in (3) vanishes. Then, inserting (1) into (3) yields

$$Q = \sum_{\mathbf{k}i} \alpha_{\mathbf{k}i}^2 \frac{1}{a^2} \sin^2(\mathbf{k} \cdot \mathbf{a}) \left[1 - \frac{(\mathbf{a} \cdot \mathbf{q}_{\mathbf{k}i})^2}{a^2} \right] . \tag{4}$$

Since static displacement has a relatively long wavelength, $\sin(\mathbf{k} \cdot \mathbf{a})$ can be approximated to $\mathbf{k} \cdot \mathbf{a}$. Thus,

$$Q \approx \sum_{\mathbf{k}i} \alpha_{\mathbf{k}i}^2 \left[\mathbf{k} \cdot \frac{\mathbf{a}}{a} \right]^2 \left[1 - \frac{(\mathbf{a} \cdot \mathbf{q}_{\mathbf{k}i})^2}{a^2} \right] . \tag{5}$$

In order to express $\alpha_{\mathbf{k}i}$ as a function of $\mathbf{k}$, it may be useful to consider dynamic displacement of atoms due to thermal vibration, which is given by

$$u_n = \sum_{\mathbf{k}i} \alpha_{\mathbf{k}i} \cos(\mathbf{k} \cdot \mathbf{a}_n - \omega_{\mathbf{k}i} t) , \tag{6}$$

where the same notation was used as in (1) with an additional time dependent term with parameters $\omega_{\mathbf{k}i}$ for a vibration frequency and t for time. Equality between the kinetic and potential energies yields

$$\alpha_{\mathbf{k}i}^2 = \frac{2k_B T}{mN\omega_{\mathbf{k}i}^2} , \tag{7}$$

where m is the mass of an atom, and N is the total number of atoms. For a small $\mathbf{k}$, a dispersion relation is approximately expressed by a linear relationship, $\omega_{ki} = v_i k$, with the wave velocity v_i as a proportional coefficient. Here the distribution of $\mathbf{k}$ is isotropic because of the initial assumption. From a relationship of elastic constants $C_i = \rho v_i^2$ with ρ being the atomic density, the dynamic displacement frequency can be described with time independent parameters as follows:

$$\omega_{ki} = k\sqrt{C_i/\rho} \ . \tag{8}$$

Then the dynamic displacement amplitude due to thermal vibration is obtained by inserting (8) into (7),

$$\alpha_{ki}^2 = \frac{2k_B T}{mNk^2} \frac{\rho}{C_i} \ . \tag{9}$$

Note that there is no time related factor in this equation. Considering static displacement as an instantaneous snap shot of dynamic displacement, it would be reasonable to use Eq. (9) for the static displacement amplitude with the following modification: The potential energy for a single mode of thermal vibration $k_B T$ is replaced by the free-energy increment due to defect accumulation. We will write it as $x\Delta f/3N$, where x is the number of defects and Δf is the free-energy increment per defect. The factor $3N$ in the denominator is to make $x\Delta f$ the potential energy for a single mode of the displacement wave, assuming that the free-energy increment is equally partitioned to each normal vibration mode. Thus, Eq. (5) becomes

$$Q = \frac{2\rho x \Delta f}{3mN^2} \sum_{ki} \frac{1}{C_i} \left[\frac{\mathbf{k}}{k} \cdot \frac{\mathbf{a}}{a} \right]^2 \left[1 - \left[\frac{\mathbf{a}}{a} \cdot \mathbf{q}_{ki} \right]^2 \right] \ . \tag{10}$$

This summation can be approximated to an integral form with continuously varying $\mathbf{k}$. For this mathematical procedure, $\mathbf{a}$ is fixed and $\mathbf{k}$ is varied by varying k and the angle θ formed by $\mathbf{k}$ and $\mathbf{a}$. The probability of finding k in a small segment $dk\,d\theta$ is $V/4\pi^2 k^2 \sin\theta dk\,d\theta$ where V is a unit-cell volume. Since the total number of $\mathbf{k}$ is N, $\mathbf{k}$ can take a value up to $\frac{1}{3}(6\pi^2 N/V)$. Also notice that $\mathbf{k}\|\mathbf{q}_{k1}$ and $\mathbf{k}\perp\mathbf{q}_{k2},\mathbf{q}_{k3}$. With all these taken into account, Q is finally given as

$$Q = \frac{4\rho x \Delta f}{45M} \left[\frac{1}{C_1} + \frac{3}{C_2} \right] \ , \tag{11}$$

where $M = mN$, a mole weight and the isotropic condition, $C_2 = C_3$, is used.

If C_i remains constant independent of x, the crystal would expand linearly to an infinite value with increasing the defect concentration because of the linearity between Q and x in the above equation. However, this is not the case, since the anharmonicity requires C_i to decrease with increasing Q. This effect of Q on C_i can be expressed by expanding $\ln C_i$ to a linear term

$$\ln C_i = \ln C_{i0} + \frac{1}{C_{i0}} \frac{\partial C_i}{\partial Q}\bigg|_{Q=0} Q \ , \tag{12a}$$

where C_{i0} is the C_i value at $Q = 0$. Then

$$C_i = C_{i0}\exp(-bQ) \ , \tag{12b}$$

where

$$b = -\frac{1}{C_{i0}} \frac{\partial C_i}{\partial Q}\bigg|_{Q=0} \ .$$

The logarithmic form was employed by Gruneisen[12] and Ida[24] for mathematical convenience and is also chosen in the present work to obtain a simple analytical expression for the crystalline instability. Other functions of C_i could be expanded to express the anharmonicity. However, the differences from (12b) can be shown to be negligible due to a small magnitude of Q of the order of 10^{-3}–10^{-2}. Thus, using various expressions of the anharmonicity has negligible effects on the final result.

When (12b) is inserted into (11), we have a similar equation to that of the thermal vibration case.

$$Q\exp(-bQ) = \frac{4\rho x \Delta f}{45M} \left[\frac{1}{C_{10}} + \frac{3}{C_{20}} \right] \ . \tag{13}$$

Variation of Q as a function of x is schematically shown in Fig. 1. It is obvious that the $Q-x$ curve has a physically reasonable meaning only along a solid line. The derivative dQ/dx becomes infinity as x approaches x^*, indicating that the lattice atoms would spontaneously separate from each other at $x = x^*$. Thus, the crystalline structure is considered to be unstable at the critical point (x^*, Q^*) that are given by

$$x^* = \frac{45M}{4eb\rho\Delta f} \left[\frac{1}{C_{10}} + \frac{3}{C_{20}} \right]^{-1} \ , \tag{14a}$$

$$Q^* = \frac{1}{b} \ . \tag{14b}$$

It should be noticed that this instability arises when increase of the strain accompanies softening of the elastic constants as described in (12b). Hence, this instability is called the elastic instability.

At the instability point, the elastic constant is obtained by inserting $Q^* = 1/b$ into Eq. (12b),
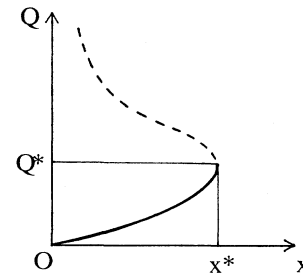
$$C_i^* = 0.37 C_{i0} \ . \tag{15}$$

FIG. 1. A schematic diagram of the strain (Q) vs defect concentration (x) relationship described by Eq. (13). Q^* and x^* are the values at the instability point.

Therefore, the elastic constant is expected to decrease by 67% for all materials when they undergo amorphization.

III. RESULTS AND DISCUSSION

Experimentally, the critical strain Q^* corresponds to the maximum value of the fractional increase of the lattice parameter observed at the onset of amorphization. Unfortunately, parameters that are necessary for calculation are available only in Si, FeTi, and NiAl to make comparison with the experimental values. Therefore, these materials are taken as representative cases to test the proposed model.

In order to calculate Q^*, the unknown parameter b is eliminated in Eqs. (14a) and (14b);

$$Q^* = \frac{4e\rho x^* \Delta f}{45M}\left[\frac{1}{C_{10}} + \frac{3}{C_{20}}\right]. \tag{16}$$

In this equation, the product $x^*\Delta f$ is a total free-energy increase at the instability point and is therefore equal to the driving force for amorphization. In the case of Si, amorphous structure has been characterized mainly by bond-angle distortion of tetrahedrally coordinated Si atoms.[25,26] Thus, $x^*\Delta f$ can be replaced by the stored energy, ΔH_s, due to the bond-angle distortion, which can be derived from the observed half width of a transverse-optical peak in a Raman spectrum. Sinke et al.[27] calculated a stored energy of 19 kJ/mol for both as-deposited and as-implanted amorphous Si by using equations given by Wong and Lucovsky[28] and Saito, Kurosawa, and Ohdomari.[29] In the case of irradiation-induced amorphization of intermetallic compounds, the chemical ordering energy has been proposed to be a major part, if not all, of the driving force.[2] Empirically,[30] the chemical ordering energy is known to be approximately $\frac{1}{3}$ of the formation enthalpy, $-\Delta H_f$, that has been experimentally determined in the case of FeTi and NiAl (Ref. 31) or can be calculated by using Miedema's formula[32] for other compounds. The elastic constants C_{10} and C_{20} in (16) are replaced by the single-crystal elastic constants C_{11} and C_{44}, respectively, and can be found in a Landolt-Bornstein table.[33] Therefore, the critical value Q^* can be calculated by the following equations:

$$Q^* = 0.24\frac{\rho\Delta H_s}{M}\left[\frac{1}{C_{11}} + \frac{3}{C_{44}}\right] \quad \text{for Si} \tag{17a}$$

$$= 0.08\frac{\rho(-\Delta H_f)}{M}\left[\frac{1}{C_{11}} + \frac{3}{C_{44}}\right],$$

$$\text{for FeTi and NiAl.} \tag{17b}$$

Table II lists the calculated value of Q^* and parameters used for the calculation. The critical strain Q^* can be compared with the maximum lattice parameter increase $\Delta a/a_0^*$, observed experimentally during the amorphization process. In the case of Si and FeTi, $\Delta a/a_0^*$ is equal to or larger than the Q^* and amorphization was observed. On the contrary in NiAl, $\Delta a/a_0^*$ is only $\frac{1}{3}$ of the Q^* and the crystalline structure was found to be stable under the irradiation condition. Thus, the critical strain criterion for the elastic instability of crystals are found to well describe the amorphization mechanism.

As shown earlier in Table I, all compounds that undergo amorphization exhibit more than 40% decrease in the shear elastic constant, while others exhibit only 10–20% decrease. This tendency agrees qualitatively with the proposed model that predicts a 67% decrease of the shear elastic constant for all amorphized materials. The quantitative difference may be partly due to the simple assumption of the elastic isotropy in the theory despite that the elastically anisotropic polycrystalline specimens were used for the experiment. (A Zener's anisotropy factor,[34] C_{44}/C', is 0.67 for FeTi and 3.34 for NiAl. A large anisotropy for NiAl is mainly due to a premartensitic effect near room temperature, showing a substantially soft C'.[35,36]) In an anisotropic crystal, one shear elastic constant decreases more than the other. In a polycrystalline form of such a crystal, a measured shear elastic constant takes a statistically averaged value of C' and C_{44} that may be given, for example, by the Reuss average,[37]

$$G_R = \frac{10C'C_{44}}{4C_{44} + 6C'}. \tag{18}$$

Because of this statistical character of the anisotropic polycrystalline materials, a large decrease of one shear elastic constant is hampered by the smaller decrease in another shear elastic constant. According to the Reuss average, 40% decrease in G_R can be observed when C' and C_{44} decrease, respectively, by 67 and 34% or 27 and

TABLE II. Calculated values of Q^* and the experimental values $\Delta a/a_0^*$. Parameters used for the calculation are also listed.

	M (g/mol)	ρ (g/cm^3)	C_{11} ($\times 10^{12}$ dyn/cm^2)	C_{44}	$-\Delta H_f$ (kJ/mol)	ΔH_S (kJ/mol)	Q^* ($\times 10^{-2}$)	$\Delta a/a_0^*$ ($\times 10^{-2}$)
Si	28.1	2.34	1.65	0.79		19.0	0.70	1.0
FeTi	51.9	6.54	3.10	0.75	31.0		1.35	1.3–2.0
NiAl	42.8	5.91	2.02	1.15	58.5		2.00	0.67

67%. Thus, the calculated value of 67% for a decrease of the shear elastic constant can be considered as a largest possible value that is observed in elastically isotropic materials. On the other hand, in anisotropic polycrystalline materials, a smaller decrease of the shear elastic constant would be observed.

IV. SUMMARY

Lattice strain and softening of the shear elastic constant were shown to be common observations during various solid-state amorphization processes in a wide range of materials. Based on these observations, the crystalline stability was theoretically evaluated by introducing static displacement of lattice atoms as a manifestation of lattice defects and by calculating the lattice strain (Q) as a function of the defect concentration (x). When the anharmonicity was taken into account, there was an instability point at which dQ/dx was found to diverge to infinity. The critical strain at the instability point was calculated for Si, FeTi, and NiAl and found to agree well with the lattice parameter increase observed before amorphization took place. The calculated elastic constant was found to decrease by 67% independent of materials, which agreed qualitatively with experiment. The quantitative differences from the experiments were attributed to the elastic anisotropy effects and the statistical nature of polycrystalline materials used for the experiment. It was concluded that solid-state amorphization takes place because of the elastic instability of the crystalline structure induced by a critical lattice strain and associated softening of shear elastic constant that are caused by static displacement of atoms from their lattice sites.

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