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CORRELATION BETWEEN THE ELASTIC-SHEAR-INSTABILITY-MECHANISM AND EMPIRICAL CRITERIA FOR IRRADIATION-INDUCED AMORPHIZATION*

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MASTER

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ABSTRACT

In an attempt to correlate the shear instability mechanism with empirical criteria for irradiation-induced amorphization, shear moduli of an A_3B-type f.c.c. crystal were calculated as a function of the chemical long range order parameter (S) using a Morse potential. The shear moduli were found to decrease with decreasing S. When the depth and the curvature of the A-B potential were changed while keeping the A-A and B-B potentials constant, the magnitude of the decrease in shear moduli is greater for deeper and narrower A-B potentials. The present results indicate that a shear instability should occur more readily in compounds with larger ordering energy and larger elastic moduli. These results agree with the reported empirical criteria for irradiation-induced amorphization, therefore providing further support for the shear instability mechanism for solid-state amorphization.

INTRODUCTION

Many intermetallic compounds have been found to be susceptible to amorphization under high energy particle irradiation. A substantial softening of the shear modulus, chemical disordering, and a large lattice dilation were observed prior to amorphization induced by ion irradiation [1,2]. These observations suggested that amorphization occurs when the crystalline lattice becomes mechanically unstable to shear stress [3]. Empirically it was also found that the compounds which undergo irradiation-induced amorphization in general have a small solubility range [4], a large difference in the atomic radii, and a large bulk modulus [5]. An explanation of these general empirical criteria for irradiation-induced amorphization can be expected in terms of the underlying shear instability mechanism.

In the present work, we have investigated the relationship between the shear instability mechanism and the empirical criteria for amorphization by calculating the softening of the shear modulus caused by chemical disordering. Since chemical disordering is a dominant phenomenon observed during irradiation [1-3], our calculation is expected to approximate the irradiation-induced softening effect. In addition, since amorphization occurs more readily with increasing softening [2,6,7], such a calculation can perhaps reveal the tendency toward amorphization for different potential shapes (different compounds). Therefore the dependence of the shear modulus softening on the potential shape can help us understand the underlying factors for amorphization, and the

correlation between the shear instability mechanism and the empirical criteria.

PROCEDURES

The calculation was performed for an A_3B-type f.c.c. compound. Considering the first and second nearest neighbor interactions, the cohesive energy of the A_3B compound is expressed by a quadratic form of the chemical long range order parameter, S,

$$\Phi(r,S) = A(r) + B(r)\ S^2 \qquad (1)$$

where

$$A(r) = 3/8(9\phi_1^{AA} + \phi_1^{BB} + 6\phi_1^{AB}) + 3/16(9\phi_2^{AA} + \phi_2^{BB} + 6\phi_2^{AB}) \qquad (1a)$$

$$B(r) = -3/8(\phi_1^{AA} + \phi_1^{BB} - 2\phi_1^{AB}) + 9/16(\phi_2^{AA} + \phi_2^{BB} - 2\phi_2^{AB}) \qquad (1b).$$

Here the first bracketed term in B(r) is generally called "the ordering energy". The parameter ϕ_z^{mn} is the cohesive energy of an m-n pair (m and n are either A or B) at the zth nearest neighbor position, for which we employed a Morse potential,

$$\phi(r) = D\ [\ \exp\{-2\alpha(r-r_0)\} - 2\ \exp\{-\alpha(r-r_0)\}] \qquad (2).$$

Here D and α are parameters determining the shape of the potential; r is the interatomic distance; and r_0 is the equilibrium interatomic distance at the first nearest neighbor position. Since

$\phi(r_0) = -D$, and $\frac{d^2\phi}{dr^2} = 2\alpha^2 D$, the parameter D reflects the depth and to a lesser extent the curvature of the potential at $r=r_0$, while α influences only the curvature.

Cu_3Au was chosen as a reference system. We employed the same parameters for Cu_3Au as those used by Roy et al. [8] which are listed in Table 1. Hypothetical compounds of the A_3B type were created by changing the shape of the A-B pair potential, with the A-A and B-B potentials kept the same as the Cu-Cu and Au-Au potentials. This was done by systematically changing the parameters (α_{AB} and D_{AB}) of the A-B pair. Figure 1 illustrates the variation of the A-B pair potential for various values of α_{AB} (Fig. 1a) and D_{AB} (Fig. 1b). As expected, the potential becomes narrower and deeper with increasing α_{AB} and D_{AB}. The effect of D_{AB} on the curvature is significantly less than that of α_{AB}.

The elastic constants, C_{ij}, were calculated by taking the second derivative of $\Phi(r,S)$ with respect to strain, ε,

$$C_{ij}(r,S) = \frac{d^2A(r)}{d\varepsilon_i d\varepsilon_j} + \frac{d^2B(r)}{d\varepsilon_i d\varepsilon_j} S^2 \qquad (3).$$

Here the subscripts of C and ε follow the Voigt notation, and indicate the crystallographic orientations. The detailed expression of the elastic constant calculation for a single component cubic material was given by Girifalco and Weizer [9]; their formulation was applied to derive the elastic constants of the A_3B compounds. In the present work, since we are interested in the shear moduli, C_{44} and $C' = \frac{1}{2}(C_{11}-C_{12})$ are calculated at an

equilibrium interatomic distance determined by solving $\frac{d\Phi(r,S)}{dr} = 0$ for r.

RESULTS AND DISCUSSIONS

Figure 2 shows the calculated variation of the shear moduli as a function of chemical disordering for two different A_3B compounds characterized by different sets of α_{AB} and D_{AB}. As the chemical long range order parameter decreases from 1 to 0, both C_{44} and C' decrease quadratic in S, which is consistent with the previous observation in Kr^+ irradiated Zr_3Al [3]. The relative decrease is greater for the compound with the larger shear moduli in the ordered state (dotted line) than that for the compound with the smaller shear moduli (solid line). The same results can be derived for the bulk modulus because of the isotropic pair potential characteristics.

Figure 3 shows the influence of the A-B potential shape on the net decrease of the shear moduli after complete disordering. Here, we consider a fractional decrease of the shear moduli, defined by $\frac{C(S=0)-C(S=1)}{C(S=1)}$, where C is either C_{44} or C'. This quantity is plotted in percent versus α_{AB} (Fig. 3(a)) and D_{AB} (Fig. 3(b)). Both figures show that the net fractional decrease of the shear moduli becomes greater with increasing α_{AB} and D_{AB}, i.e., in a compound with a narrower and deeper pair potential. It is obvious from Eq. (1b) that a compound with a deeper potential has a large ordering energy, hence exhibits strong tendency towards chemical ordering in the equilibrium state. A narrower potential implies a

more rapid increase in energy due to atom displacement from their equilibrium position. Since compositional deviation from stoichiometry accompanies atomic displacement due to point defect formation, the compounds with narrower potentials are likely to have a smaller solubility range in the equilibrium state. It should be noted that chemical disordering also induces atomic displacement. The net displacement is expected to be larger for a compound with large difference in the atomic radii between two consitituing elements. Once chemical disordering is introduced by irradiation, the energy increase as well as the decrease in shear moduli will be greater in compounds with a larger atomic size difference.

Therefore, our calculation indicates that a larger decrease of the shear modulus is expected in precisely those compounds which fit the empirical criteia for irradiation-induced amorphization, namely, the compounds with strong chemical ordering, large elastic moduli, a small solubility range, and a large atomic size difference. This correlation suggests that the empirical criteria have their origin in the shear instability mechanism. The compounds for which the empirical criteria predict amorphization are those which exhibit a large decrease of the shear modulus during chemical disordering.

SUMMARY

The variation of the shear modulus caused by chemical disordering was calculated using a Morse potential with different shapes. The decrease of the shear modulus during disordering was

found to be greater in compounds with a deeper and narrower potential. The results are consistent with empirical criteria for irradiation-induced amorphization, and therefore indicate that the empirical criteria for irradiation-induced amorphization originate from the shear instability amorphization mechanism.

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REFERENCES

1. L. E. Rehn, P. R. Okamoto, J. Pearson, R. Bhadra, and M. Grimsditch, Phys. Rev. Lett. **59**, 2987 (1987).

2. J. Koike, P. R. Okamoto, L. E. Rehn, R. Bhadra, M. Grimsditch, and M. Meshii, Proc. MRS Symp. **157**, 777 (1990).

3. P. R. Okamoto, L. E. Rehn, J. Pearson, R. Bhadra, and M. Grimsditch, J. Less-Comm. Metals **140**, 231 (1988).

4. J. L. Brimhall, H. E. Kissinger, and L. A. Charlot, Rad. Effects **77**, 237 (1983).

5. M. Nastasi, D. Lilienfeld, H. H. Johnson, and J. W. Mayer, J. Appl. Phy. **59**, 4011 (1986).

6. P. R. Okamoto and L. E. Rehn, unpublished results. Also see, P. R. Okamoto and M. Meshii, in *Science of Advanced Materials*, eds. by H. Wiedersich and M. Meshii (American Society of Metals, Metals Park, Ohio), in press.

7. M. Grimsditch, K. E. Gray, R. Bhadra, R. T. Kampwirth, and L. E. Rehn, Phys. Rev. B **35**, 883 (1987).

8. D. Roy, A. Manna, and S. P. Sen Gupta, J. Phys. F: Metal Phys. **2**, 1092 (1972).

9. L. A. Girifalco and V. G. Weizer, Phys. Rev. **114**, 687 (1959).

TABLE AND FIGURES

Table 1 The parameters for the Morse potential of Cu_3Au, employed as a reference system (after Roy et al. [8]).

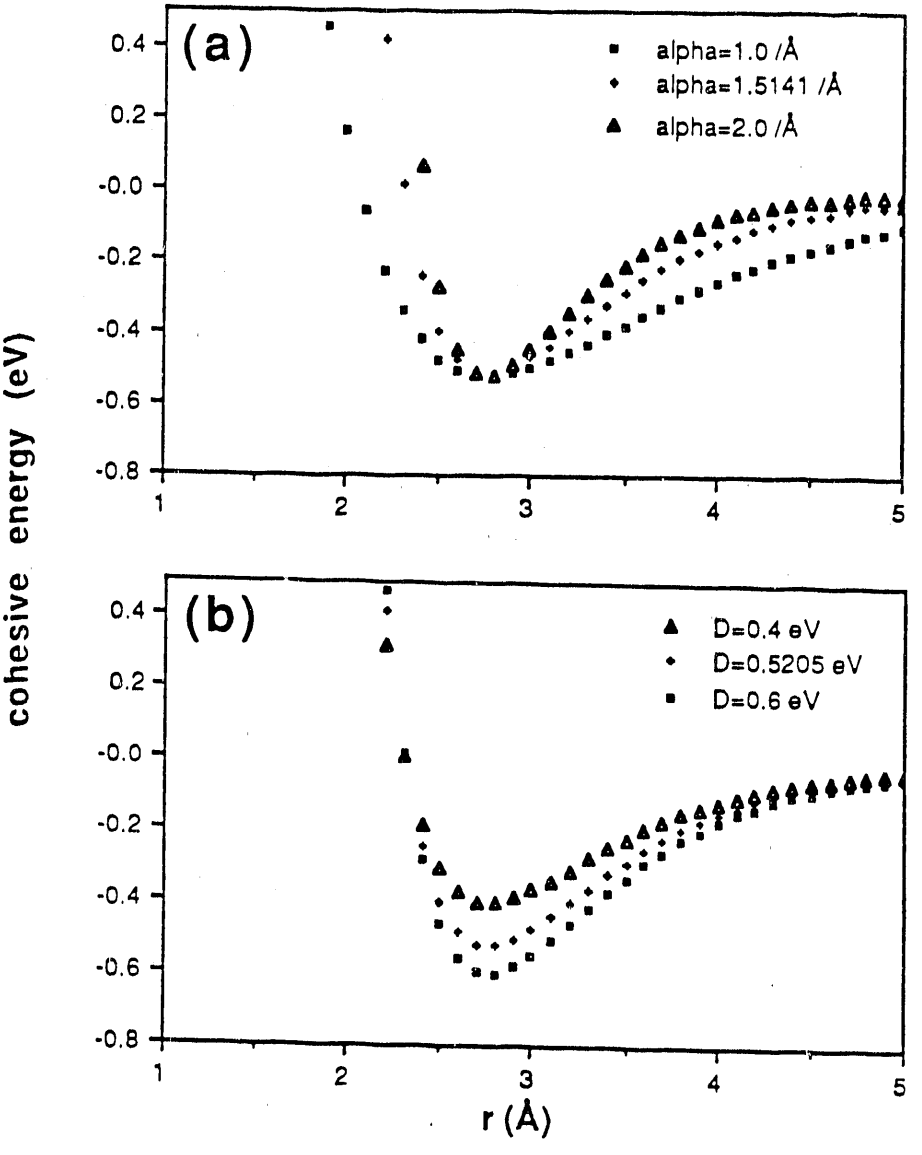
Fig.1 The variation of the A-B pair potential for various values of α_{AB} and D_{AB}. In (a), α_{AB} is varied with fixed values of D_{AB}=0.5205 eV and r_0=2.7621. In (b), D_{AB} is varied with fixed values of α_{AB}=1 5141 $Å^{-1}$ and r_0=2.7621 Å.

Fig.2 The Variation of the shear moduli, C' and C_{44}, with decreasing the chemical long range order parameter S. The solid lines are for D_{AB}=0.5205 eV and α_{AB}=1.514 $Å^{-1}$. The dotted lines are for D_{AB}=1.0 eV and α_{AB}=3.0 $Å^{-1}$.

Fig.3 The fractional decrease of the shear moduli caused by complete chemical disordering as a function of (a) α_{AB} with fixed values of D_{AB}=0.5205 eV and r_0=2.762, and of (b) D_{AB} with fixed values of α_{AB}=1.5141 $Å^{-1}$ and r_0=2.7621 Å.

Table 1

atom pair	D (eV)	α ($Å^{-1}$)	r_o (Å)
Au-Au	0.5566	1.6300	2.9214
Cu-Cu	0.4867	1.3980	2.6230
Au-Cu	0.5205	1.5141	2.7621


(a)
alpha=1.0 /Å
alpha=1.5141 /Å
alpha=2.0 /Å
(b)
D=0.4 eV
D=0.5205 eV
D=0.6 eV
cohesive energy (eV)
r (Å)
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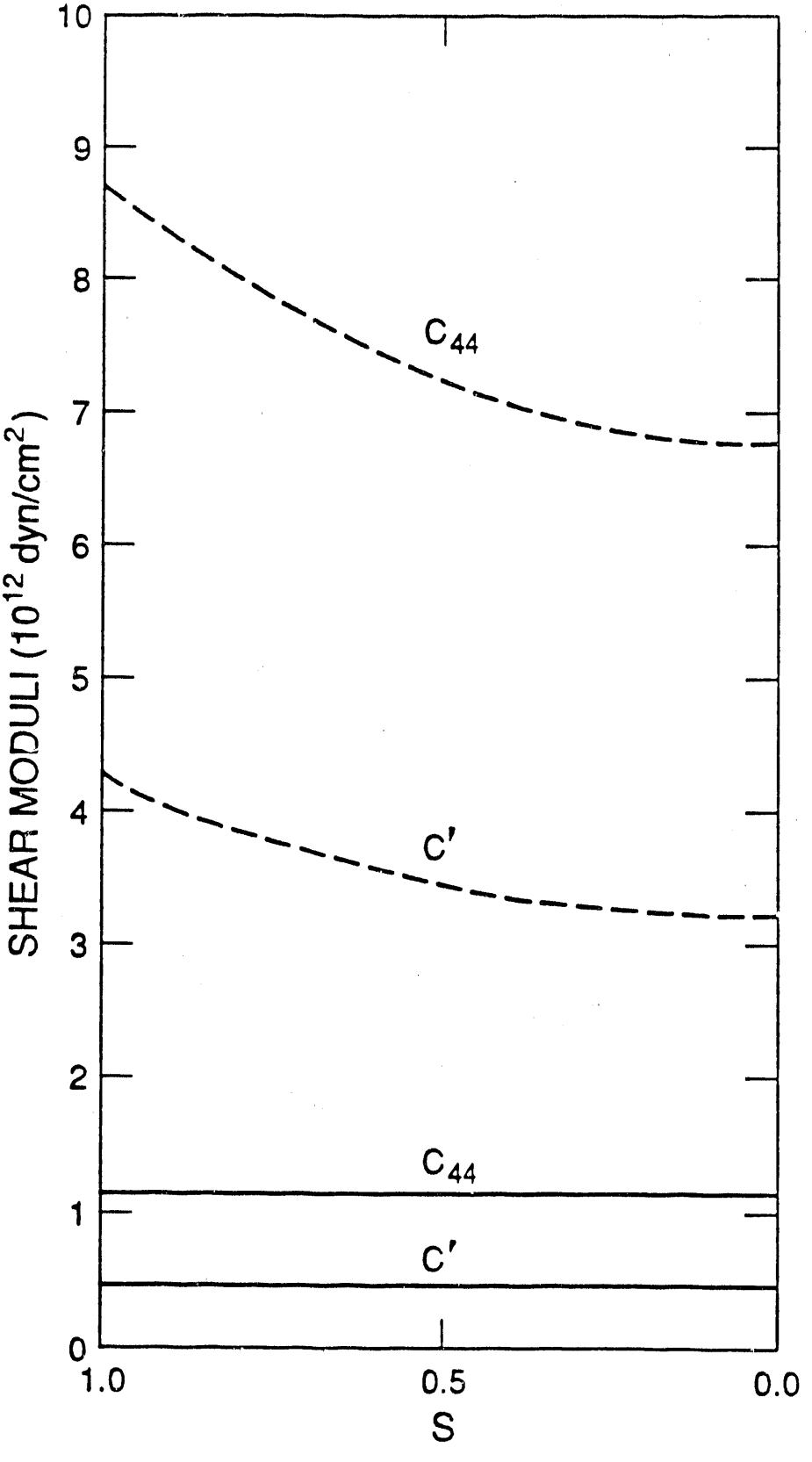
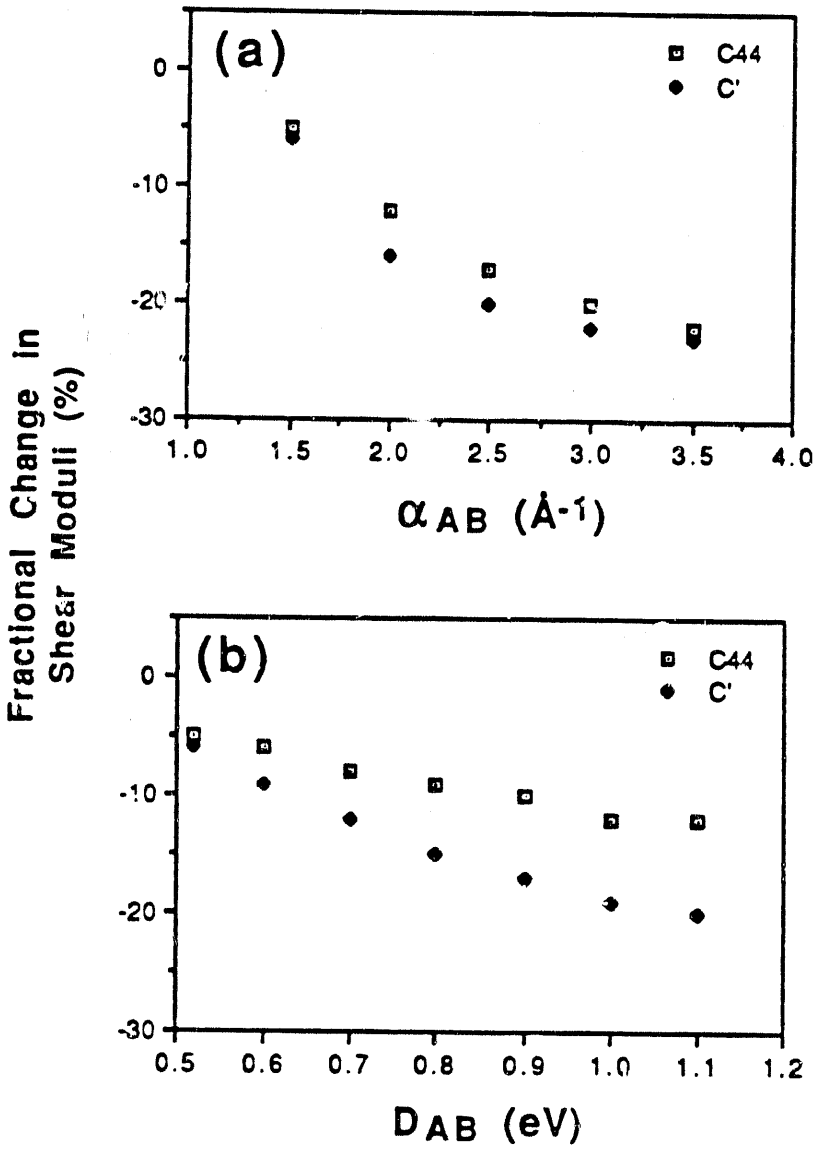
0.2
-0.0
-0.2
-0.4
-0.6
-0.8
1
2
3
4
5


10
9
8
7
6
5
4
3
2
1
0
SHEAR MODULI (10^{12} dyn/cm^2)
C_{44}
C′
C_{44}
C′
1.0
0.5
0.0
S


(a)
C44
C'
0
-10
-20
-30
1.0
1.5
2.0
2.5
3.0
3.5
4.0
α_{AB} (Å^{-1})
(b)
C44
C'
0
-10
-20
-30
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
D_{AB} (eV)
Fractional Change in Shear Moduli (%)

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