

The role of chemical disorder and volume expansion in crystal-to-amorphous transitions: simulation results for NiZr₂ and Cu₃Au

Vittorio Rosato

ENEA C.R.E. Casaccia, Progetto Materiali Metallici Innovativi, 00100 Rome (Italy)

Carlo Massobrio

Ecole Polytechnique Fédérale de Lausanne, Institut de Physique Expérimentale, CH-1015 Lausanne (Switzerland)

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Abstract

We report the results obtained in a molecular dynamics simulation study of the behavior of two different systems, NiZr₂ and Cu₃Au, subjected to a chemical disordering process, under different thermodynamical conditions. We underline the relevant phenomena which, in the first case, trigger the onset of the crystal-to-amorphous transition but in the latter do not. We focus on the dominant role played by volume expansion and elastic softening as precursor effects on the onset of the transition. Finally we draw attention to the percolation model (C. Massobrio and V. Pontikis, *Phys. Rev. B*, 45 (1992) 2484) which correlates elastic instability to percolation of locally expanded regions located around the defects.

1. Introduction

The growing technological relevance of metallic amorphous materials has transmitted an important impulse to the study of crystal-to-amorphous (hereafter c-a) transitions. The main goal of current research in this field is to understand to what extent different techniques, which are employed to induce the c-a transition, could be related to a common microscopic mechanism. Processes such as hydrogen absorption [1], electron [2] or ion irradiation [3], plastic deformation of pure elements [4, 5] and solid state interdiffusion [6] involve an increase in energy of the solid up to the point at which it becomes unstable with respect to its parent crystalline state. Several mechanisms have been proposed to account for the energy storage and the subsequent amorphization. In this paper we intend to focus mainly on two of these, namely "volume expansion" [1] and "chemical disorder" [2].

2. Volume expansion

As expressed in a review paper of 1986, Cahn and Johnson [7] view solid state amorphization and melting as manifestations of the same first-order phase transitions. In relation to this interpretation, much work has been performed since then to prove the existence of an elastic instability which could lead to homogeneous

nucleation of the disordered phase, just as occurs at the melting point in the absence of extended defects.

In 1987 Rehn *et al.* reported a large (50%) softening of the shear elastic constant on ion-irradiated samples of Zr₃Al [8]. The extrapolation to zero of the shear elastic constant as a function of the lattice dilation indicates that the disordered crystal becomes unstable with respect to small density fluctuations and, therefore, the transition is apparently triggered by an elastic instability. Moreover, the behavior of the elastic constants in irradiated samples looks very much like that observed in different materials heated up to melting [9].

These convictions have been strengthened by experimental evidence of transitions to the amorphous state in hydrogenated samples, where large lattice expansions are achieved without introducing a high concentration of point defects or chemical disorder and a c-a transition occurs at a volume dilation of $\Delta V/V = 2.4\%$ [1]. On the theoretical side Wolf *et al.* conjectured that lattice expansion is the fundamental physical response of a system driven far from equilibrium and its destabilizing effect depends on its magnitude more than how it is produced [10]. We shall come back to this intriguing point shortly.

3. Chemical disorder

Chemical disorder consists of the loss of the regular chemical arrangement of the atoms in the lattice. It

can be achieved either on a long-range scale through the formation of stacking faults which destroy the long-range order sequence, or on a smaller scale by the creation of antisite defects which consists in removing an atom from its regular lattice site and exchanging its position with that of an atom belonging to a different species. These disordering processes are likely to occur under ion or electron irradiation of alloys through the random recombination of vacancy–interstitial pairs and/or replacement collision sequences.

Luzzi *et al.* [11, 12] proved that a certain level of chemical disorder is needed to establish a topological disorder, *i.e.* to attain an amorphous structure. This hypothesis stands on the observation that amorphous regions start nucleating at dislocations or grain boundaries [13] where chemical disorder is readily achievable. Two competing processes intervene during electron irradiation: irradiation-induced disordering and thermal reordering. The maximum degree of disorder will thus be related to the interplay between these two effects. At low temperatures, irradiation produces an effective chemical disorder, owing to the low efficiency of the reordering mechanism. In the high temperature range, in turn, the irradiation effects are greatly reduced owing to fast defect migration. Pioneering molecular dynamics (MD) work on NiZr_2 gave support to the hypothesis that chemical disorder is the main driving force of the c–a transition [14, 15]; these findings were followed later by simulation work on different alloys and the role played by chemical disorder was often questioned [16]. In order to introduce further elements for debate on this topic, we present here a combined set of MD simulations with the aim of comparing the behavior of two systems, NiZr_2 and Cu_3Au , which are representative of two different classes of alloys. This paper reviews published data and includes new results for NiZr_2 , a line compound which melts before disordering and undergoes a c–a transition by several means [17, 18]. Cu_3Au is, in turn, a compound with a much larger stability region in the phase diagram. Furthermore, it exhibits a disordered phase at a temperature $T_c = 663$ K equal to about half the melting temperature [19]. Because of these features we believe a c–a transition is unlikely to take place, even at temperatures lower than T_c . The comparative analysis of the behavior of these two systems will provide useful insights to highlight the role played by the different processes in triggering the c–a transition.

4. Model and computations

Both systems were modeled using an empiric interatomic potential derived from a tight-binding scheme, based on the second-moment approximation of the

electronic density of states. The model, extensively described elsewhere [20–22], has been shown to reproduce with good accuracy bulk and defect properties of most transition metals with f.c.c. and h.c.p. structures [21, 22] and those of several alloys [14, 22]. Using a suitable cut-off distance for interactions, it is possible to reproduce satisfactorily the thermodynamical behavior of those systems up to the melting point. With respect to the fitting procedure we point out that the cross parameters in the interatomic potential are fitted to cohesive energy, elastic constants, equilibrium condition and the latent heat of mixing of the alloy, while the parameters describing the interaction between atoms of the same species are fitted to analogous properties of the pure metals [14, 22]. In the case of Cu_3Au , however, an additional condition, namely the stability at $T = 0$ K of the chemically ordered phase with respect to the introduction of an antisite defect, was used. The introduction of this further condition allows correct reproduction of the order–disorder transition, which was detected by means of a direct computation of the free energy [22]. A good compromise between accuracy and computing time was reached by using a cut-off distance for the interactions which includes the fifth-neighbors shell. Simulations were carried out using the Nose–Andersen constant pressure, constant temperature technique (for the fixed pressure simulations) and in the canonical ensemble for the fixed volume simulations [14]. A fifth-order predictor-corrector algorithm with a time step of 10^{-15} s was adopted throughout our simulations. The crystalline structure of NiZr_2 is a C16 type (tetragonal structure with lattice parameters $a = 0.6843$ nm, $c = 0.5267$ nm). Each nickel atom has eight zirconium atoms and two nickel atoms as nearest neighbors, the latter at a distance $d(\text{Ni–Ni}) = c/2$ forming a linear chain. Each zirconium atom has four nickel atoms as nearest neighbours and 11 zirconium atoms disposed at four slightly different distances [23]. We used systems of $N = 144, 324$ and 768 atoms. The Cu_3Au structure is L12 (f.c.c. lattice with lattice parameter $a = 0.3737$ nm). Each gold atom has 12 copper atoms as nearest neighbors, while copper atoms have four gold atoms and eight copper atoms as first neighbors. We used a system of $N = 500$ atoms.

We will describe the results obtained in both cases, concerning the behavior of the system, upon introduction of an increasing number of antisite defects in the system. Although some authors [16] have argued that the occurrence of the c–a transition could depend critically on the introduction rate, we have not obtained any evidence to support this dependence. Antisite defects were, therefore, introduced either one by one or simultaneously and we assume that the final equilibrium state does not depend on the introduction rate.

4.1. NiZr₂

We explored the possibility of amorphizing this system by several means. First of all, we followed the response to the introduction of antisite defects, at fixed pressures, namely $P_1=0$, $P_2=160$ kbar and $P_3=240$ kbar. At each pressure, we first thermalized the system at $T=300$ K and subsequently introduced a suitable number of antisite defects to obtain a given value of the Bragg Williams order parameter S [24]. We have drawn in Figs. 1–3 the enthalpy behavior as a function of the order parameter S for the three cases. In these figures a reference value of enthalpy of the amorphous phase obtained by rapid quenching of the melt is reported for comparison. A critical value for the order parameter S_c can be obtained from these data by taking the value of S that corresponds to the first intercept with the reference enthalpy of the amorphous phase. Starting from S_c , the system enthalpy reaches the value equivalent to that of an amorphous structure. Complete amor-

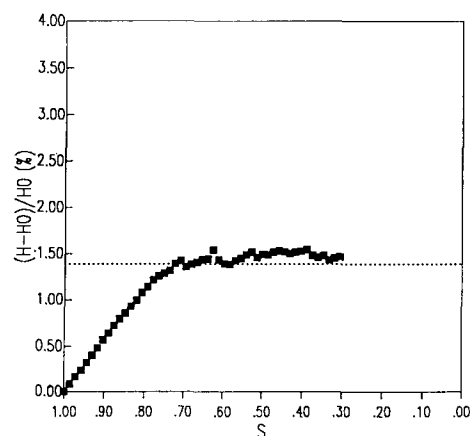


Fig. 1. Enthalpy variation, with respect to the crystalline phase, of NiZr₂ as a function of the order parameter S at $T=300$ K and $P=P_1=0$.

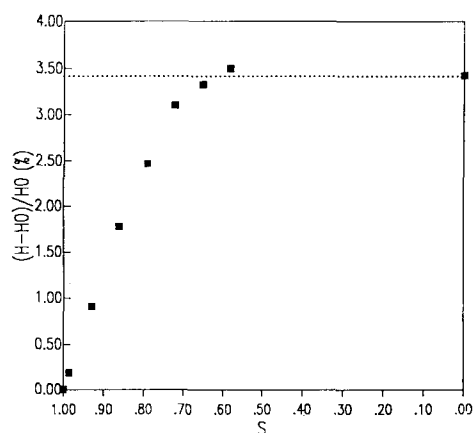


Fig. 2. Enthalpy variation, with respect to the crystalline phase, of NiZr₂ as a function of the order parameter S at $T=300$ K and $P=P_2=160$ kbar.

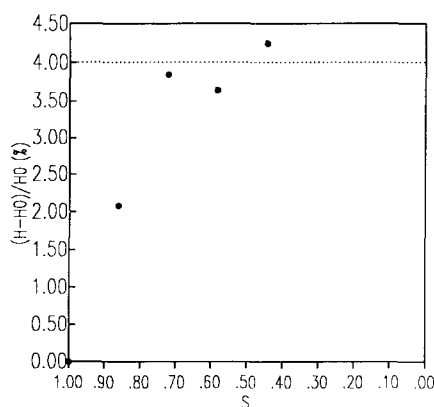


Fig. 3. Enthalpy variation, with respect to the crystalline phase, of NiZr₂ as a function of the order parameter S at $T=300$ K and $P=P_3=240$ kbar.

phization is, however, only achieved for smaller values of S [25]. S_c is thus intended to be a signature of the beginning of the transition and appears to be only weakly dependent on the external pressure.

Further evidence of the intervened c-a transformation is given by comparison of the different radial distribution functions which are discussed in detail for the case of NiZr₂ at $P=0$, in ref. 15. As it has been previously stressed, the critical value S_c corresponds only to the onset of the transition. In fact, at this value of order parameter, the system still retains a part of its crystalline phase, as the intensity of particular reflections typical of crystalline order are still present [25, 26]. This more convincing argument on the issue of the progressive behavior of the c-a reaction was introduced by Massobrio [26] by evaluating the structure factor of NiZr₂, along different directions, for several values of S . In the case $P=P_1$, the structure factor at $S=0.5$ shows the persistence of Bragg peaks, even if strongly smeared out, although the system enthalpy has already reached the amorphous value (see Fig. 1). These peaks disappear completely at $S=0$. This finding is consistent with the presence in the sample of a mixture of crystalline and amorphous regions, as suggested [27] to explain the coexistence of weak Bragg peaks and diffuse rings commonly observed in diffraction patterns.

In all simulations at fixed pressure, we found that the largest volume expansion is around 2% and it increases with decreasing external pressure. At zero pressure the c-a transition gives $\Delta V/V=2.06\%$; in contrast we have $\Delta V/V=1.8\%$ for P_1 and $\Delta V/V=1.48\%$ for P_2 . Once the system reaches this value, its enthalpy and structure are compatible with that of an amorphous phase.

The case of simulations at constant volume deserves further comments since volume expansion has been invoked as a main factor responsible for the c-a transition [10]. For this computation we used a system with

initial volume at the zero pressure value for $T=300$ K. In this case, the introduction of antisite defects causes an increase in internal pressure. Figure 4 shows the behavior of the variation in internal energy with respect to the crystalline phase (under the same thermodynamical conditions) *vs.* the order parameter S . Pair distribution functions show that, even at constant volume, NiZr_2 can be amorphized, either by melt quenching or by the introduction of chemical disorder, as shown in Figs. 5 and 6. In this case, where any possible effect induced by volume expansion has been purposely suppressed, the main role is played by the internal strains which develop in the vicinity of the defective regions. As will be explained in the following, their effects will be to increase both the energy stored in the defects and their associated volume.

4.2. Elastic behavior

Mechanical instability has been invoked as the primary cause of the lattice destabilization leading to the ap-

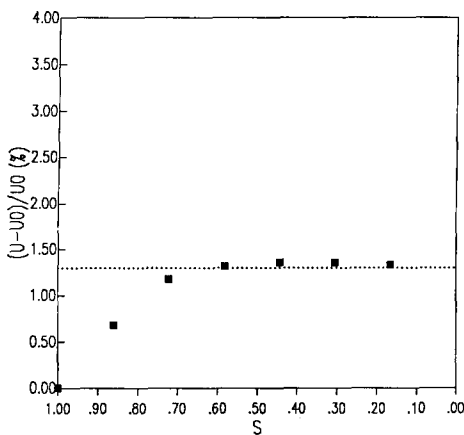


Fig. 4. Internal energy variation, with respect to the crystalline phase, of NiZr_2 as a function of the order parameter S at $T=300$ K and constant volume.

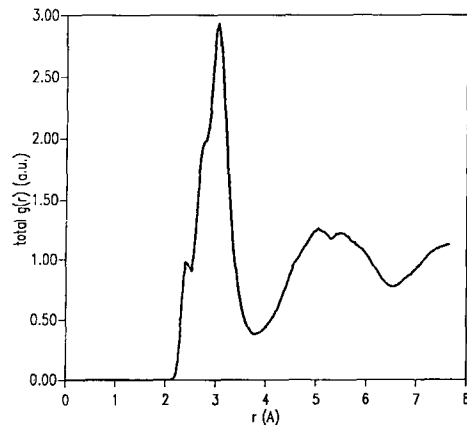


Fig. 5. Total radial distribution function at $T=300$ K and constant volume for the amorphous alloy obtained from liquid quench.

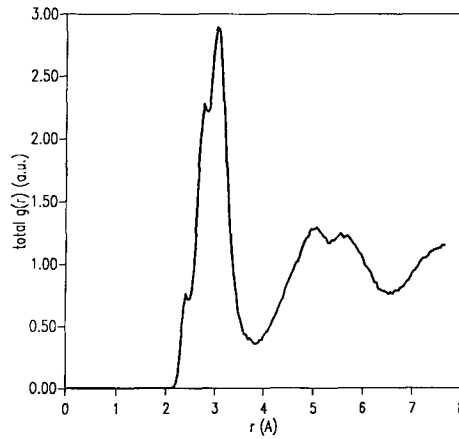


Fig. 6. Total radial distribution function at $T=300$ K and constant volume for the chemically disordered solid, $S=0.17$.

pearance of the amorphous structure. Experiments on Zr_3Al [3] have shown that the onset of the c-a transition can be induced either by hydrogen adsorption or by ion irradiation and it occurs, in both cases, at the same lattice dilation. Lattice expansion has therefore been used as a common measure of the crystal instability induced by different external perturbations, thereby establishing a tentative parallel between amorphization and melting. As a measure of the mechanical instability induced by volume expansion, the authors of ref. 3 have observed that the shear constant of Zr_3Al , although highly reduced, remains finite at the amorphization threshold. This difference has been explained in terms of polycrystalline shear, a quantity more suited to be compared with the experimental elastic constant and typically larger than the single shear constant which vanishes when the lattice collapses [10]. These facts have been interpreted as an indication that amorphization processes may be driven by a mechanical instability induced by lattice dilation, much in the same way as melting.

The aim of the detailed calculation of elastic constants, which has been recently performed [25, 26], was to verify whether the elastic instability could trigger the onset of the transition in a chemically disordered system and whether it could be considered as a precursor effect for amorphization. The computation focused on the shear elastic constants C' , C_{44} and C_{66} , for a system which exhibits tetragonal symmetry in the [001] direction. These quantities are the eigenvalues of the elastic matrix C closer to the boundary of the elastic instability region defined by $\det C=0$.

By looking at the behavior of a system homogeneously expanded without introducing defects at room temperature, it was found that the behavior of the minimal elastic constants driving isothermal and isobaric expansion are indeed quite similar up to a value $\Delta V/V=0.08$ (Fig. 7). The analogies between the c-a tran-

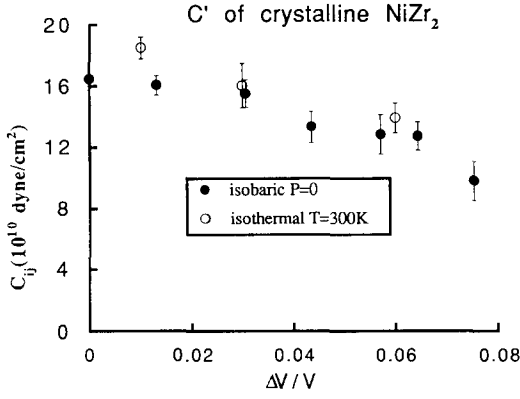


Fig. 7. Volume dependence of C' in crystalline NiZr_2 .

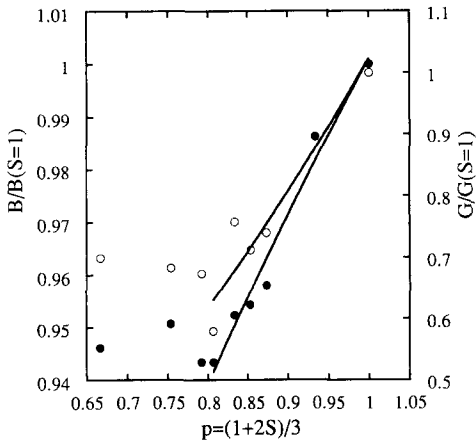


Fig. 8. Normalized average shear G (\circ) and bulk modulus B (\bullet) as a function of the probability p of finding a nickel atom on its original lattice site. The two curves are fits to power laws.

sition and melting break down in the case of isothermal dilation, since a volume expansion of 25% is needed to induce mechanical failure of the system [28]. This reveals that volume expansion alone cannot be considered responsible for the c - a transition, in agreement with the simulations at constant volume discussed in the previous section.

Voigt averaged bulk and shear moduli were evaluated as a function of the chemical order parameter S , displayed in Fig. 8 for the case $P=P_1$. By fitting the data to a power law of the form $(S-S_c)^\alpha$ for $S > 0.7$, we obtained values of the exponent $\alpha=1.23$ and 1.39 for bulk and shear constants respectively. A value of $S_c=0.688$ was found in both cases. This agrees with the previous estimate $S_c < 0.7$ obtained on the basis of thermodynamical and structural data. For the other cases ($P=P_2$, $P=P_3$ and V constant), the critical value of the order parameter S_c was defined by simply taking the value of the first intercept of the enthalpy curves with the reference value of the amorphous state obtained by melt quenching (see Figs. 1–4).

4.3. Percolation model

The speculation that softening of the elastic constants could be attributed to the presence of highly distorted regions in the lattice is based on the observation that large relaxations of the matrix, reaching up to 13% at the second neighbors distance, establish around the antisite defects in NiZr_2 [25]. This finding suggests that the variation of C' in the vicinity of S_c could be induced by the percolation of such “distorted” regions and allows the recovery, within the limits of a qualitative model, of the critical value of the order parameter as the value where percolation takes place. The idea is based on the picture of a system which, at low levels of disorder (high values of S), can be thought of as a solid solution containing impurities. Under this hypothesis, the elastic model for dilute solutions can be reasonably applied [29, 30]. The elastic energy E_{el} stored in the system can thus be written as

$$E_{el} = W_0 c (1 - c) \quad (1)$$

where W_0 is the elastic energy contained in a single impurity (in our case antisite defect) and c is the volume fraction of the impurities. E_{el} is evaluated on the basis of our simulation results by subtracting the equilibrium enthalpy of the system at a given value of S from the enthalpy of the ordered ($S=1$) system. The value of c can be expressed, in terms of the model characteristics, as follows:

$$c = \frac{n_d v_d}{N_T v_0} = \frac{2}{3} (1 - S) \frac{v_d}{v_0} \quad (2)$$

where n_d , N_T , v_d and v_0 represent respectively the number of antisite defects, the total number of molecules contained in the system, the effective molar volume of antisite defects and the molar volume associated with the perfect crystal. If we substitute eqn. (2) into eqn. (1), we obtain

$$E_{el} = -\frac{4}{9} W_0 \chi^2 (1 - S)^2 + \frac{2}{3} W_0 \chi (1 - S) \quad (3)$$

By fitting the obtained E_{el} values as a function of S to the parabola of eqn. (3), the values of W_0 and c can be determined. Using these values, it is possible to obtain the volume fraction c corresponding to the values of S_c found on the basis of the enthalpy curves. The results are shown in Table 1 and reveal that, on the basis of the percolation model, amorphization at constant volume and constant pressure can be treated on the same footing as processes induced by a sufficiently high concentration of defective regions. Table 1 recalls the positive correlation which has been found between the elastic energy associated with the single defect and the size of the volume affected by the defect with the occurrence of the transition.

TABLE 1. Summary of the data obtained by fitting the elastic energy stored in the system as a function of the order parameter using eqns. (1) and (2) (see text).

System	Conditions	W_0 (eV mol ⁻¹)	χ	S_c	c
NiZr ₂	$P=P_1$	0.92	1.139	0.688	0.24
NiZr ₂	$P=P_2$	1.81	1.640	0.65	0.38
NiZr ₂	$P=P_3$	1.67	1.574	0.70	0.31
NiZr ₂	V constant	0.98	1.244	0.722	0.23

The case of absence of the c-a transition (as for Cu₃Au) can also be explained on the basis of the percolation model, as the low distortions associated with the antisites do not allow for percolation to take place even at low values of the order parameter [22]. In fact, eqn. (4) fitted to the corresponding data of Cu₃Au, gives a value of χ smaller than unity ($\chi=0.84$) and a value of W_0 as low as 0.09 eV mol⁻¹. In the picture of the elastic model of percolation, the system behaves as if the associated volume of the defects shrank with respect to the equilibrium volume, the associated elastic energy being vanishingly small. Under these conditions, percolation of distorted regions cannot be attained and no critical value of S is achieved.

4.4. Cu₃Au

The case of Cu₃Au is very different from that of NiZr₂, as the former has a thermal behavior which allows the crystalline ordered phase to become chemically disordered at $T=663$ K. The crystal structure is much less compact than that of NiZr₂, having, at $T=300$ K, a free volume ratio V_0/V_T of 0.569 against 0.932 for NiZr₂. These values are calculated by taking for V_0 the volume occupied by the atoms considered to be hard spheres and for V_T the total volume of the system. Cu₃Au can easily be amorphized by quenching, making use of the fast quench rates allowed by molecular dynamics simulation. However, the system crystallizes easily even for high quench rates. Following a quench from $T=2500$ K down to $T=700$ K in a few picoseconds, the system relaxes into a crystalline (disordered) structure after 10^{-10} s. We only succeeded in obtaining a stable amorphous structure, within the timescale of our simulations, by quenching directly down to $T=300$ K. Once again we found a volume expansion with respect to the crystalline phase of 2% [22].

Antisite defects were introduced in the crystal at $T=300$ K and its behavior was compared with that of the amorphous phase obtained by melt quenching at the same temperature. The results are sketched in Fig. 9. The enthalpy of the glassy phase is much higher than that attainable even upon complete disordering of the chemical arrangement of the lattice.

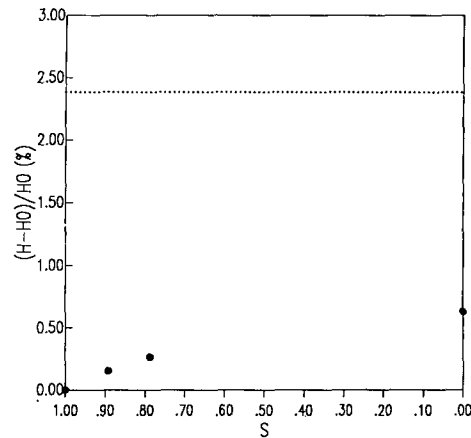


Fig. 9. Enthalpy variation, with respect to the crystalline phase, for Cu₃Au vs. S , at $T=300$ K. The dotted line represents the enthalpy of the amorphous phase, obtained by melt quenching, at the same temperature.

5. Discussion

In order to analyze the results, we focus on the main differences between the two classes of alloys considered. The first concerns the values of the latent heat of mixing which, for the case of NiZr₂, is of the order of $\Delta H_{\text{mix}}=0.39$ eV per atom [31], while in the case of Cu₃Au one has $\Delta H_{\text{mix}}=0.043$ eV per atom [32]. This is equivalent to saying that the first system is able to store a huge amount of energy in the form of chemical disorder, while the second is not. The elastic energy stored in the defects induces large distortions of the lattice which allow, at a given value of S , the percolation threshold to be reached. This result is consistent with the first empirical criterion for amorphization, expressed by Cahn and Johnson [7], stating that a large mixing enthalpy is a necessary prerequisite in solid state amorphization processes.

Another interesting piece of evidence concerns the role of volume expansion. In both cases we have found that the volume increase between crystalline and amorphous structures is always larger than 1.5%, when simulations are carried out at fixed pressure. In the case of NiZr₂ this value is attainable upon introduction of chemical disorder. In the case of Cu₃Au, in turn, because of the more open structure, the effective volume associated with the antisite defect is quite low and we were not able to induce the c-a transition by chemical disorder. Even at $S=0$ the equilibrium volume is only 1% larger than that of the corresponding crystalline ordered phase as opposed to the 2% increase required for the amorphous phase.

The picture which emerged from these results relates the occurrence of the c-a transformation to the destabilizing effect of an elastic softening. Although it has been suggested that this softening could be complete,

leading to a fascinating analogy between c-a transition and melting, we have not obtained such evidence. Our model suggests that the elastic softening of C' triggers the onset of the transition which begins when the long-range order parameter S attains a critical value. At this value of S , the concentration of *disordering defects* (in our case antisite defects but, in general, they can be generic species, such as interstitials, Frenkel pairs etc.) corresponds to a threshold for the percolation of the strained regions around the defects. Upon further introduction of defects, the systems tends to restore its elastic behavior while complete amorphization is being accomplished. At isobaric conditions the overall process is accompanied by a critical dilation of 2% but volume expansion alone cannot be considered either as a necessary or as a sufficient prerequisite for the c-a transformation to occur.

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