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Phase evolution of highly immiscible alloys under shear deformation: Kinetic pathways, steady states, and the lever-rule

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ABSTRACT

Phase evolution of dilute, highly immiscible, Cu alloys (Cu-Nb, Cu-V, and Cu-Ta) during low-temperature severe plastic deformation was investigated using large-scale molecular dynamics simulations. At low solute concentrations, each system maintained a FCC structure in steady state, but as the concentration was increased above a saturation limit (0.3 at.% for Ta, 1 at.% for Nb and 5 at.% for V), the system became two-phase, comprising co-existing FCC and amorphous phases. Unlike Cu-Nb and Cu-V, the amorphous phase in the Cu-Ta system showed strong solute partitioning. Increasing the solute concentration above a second phase boundary (8 at.% V, 9 at.% Nb, and 24 at.% Ta) led to complete amorphization. Throughout the two-phase region, the compositions of the FCC and amorphous phases remained nearly constant, thus following the lever rule. Initiating the systems either as a FCC homogeneous alloy, or with a BCC sphere embedded in a Cu matrix, had no effect on the steady state microstructure, implying uniqueness of the steady state under low-temperature shear deformation. Lastly, chemical order and phase partitioning in the amorphous Cu-Ta system under low-temperature shear is found remarkably similar to that in the equilibrium structure above the melting temperature.

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1. Introduction

Severe plastic deformation (SPD) of metal alloys during ball milling [1], accumulative roll bonding [2], or high pressure torsion [3] often leads to homogenization of alloy components, generally referred to as mechanical alloying [4]. Homogenization is even observed in immiscible alloys, such as Cu-Ag, Cu-Fe, Cu-Co and many others [1]. Various mechanisms for this homogenization process have been suggested, see for example refs [5–9,40], although a unified understanding of this process remains controversial. Some immiscible alloys, such as Cu-Ta [10], Cu-Nb [11], Cu-Mo [12,13], Ni-Ag [14] and Fe-Ag [41], on the other hand, fail to homogenize during SPD, even when shear strains are extremely high and shearing temperatures very low. Common to many of these alloys is a high heat of mixing, $\Delta H_m > 0.2$ ev/atom, at the equimolar solution, and it has been suggested from molecular dynamics [15] and molecular statics computer simulations [16] that chemical interactions bias the relocation of atom during shearing, preventing complete homogenization. These past simulation studies, however, reported on short range ordering during shear in modestly immiscible alloys and did not reveal the two-phase coexistence found experimentally in systems with very high heats of mixing. It has also been suggested that the large difference in the strengths of the two immiscible phases might also contribute to the lack of homogenization [17]. An interesting observation regarding the shear-induced mixing of these highly immiscible alloy systems is that while they do not homogenize during extended ball milling or high pressure torsion (HPT), the length scale of the phase-separated phases decreases dramatically from their initial values, from several hundreds of nanometers or more, to some tens of nanometers [18,19]. For dilute Cu-Nb alloys, new studies [20] using HPT have further revealed that the same approximate microstructure evolves whether the initial state of the system is a two-phase alloy containing large Nb precipitates or a homogeneous solid solution. These results suggest that the Cu-Nb alloy self-selects a length scale during low-temperature shear, independent of its initial state. At present there are no detailed models explaining the behavior of these strongly immiscible alloys under low temperature shear deformation. Curiously, however, this behavior is

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reminiscent of low-temperature particle irradiation of strongly immiscible Cu alloys [21]. For example, irradiation of dilute Cu-W alloys [22] results in a large supersaturation of W in Cu, ~1.5 at.%, and narrow size distribution of W precipitates, both of which being independent of the initial state of the system. In this case the controlling mechanisms have been attributed to a dynamical competition between energetic (random) recoil mixing of atoms and solute agglomeration within local melt zones in energetic displacement cascades, i.e. thermal spikes. While these two irradiation mechanisms are clearly not involved in shearing, we will show that a corresponding dynamical competition occurs during low temperature shearing. The present paper thus explores self-organization behavior in highly immiscible Cu alloys during shear deformation using large-scale molecular dynamics simulations. Three alloys are selected for study, Cu-Nb, Cu-Ta, and Cu-V; while they all have large positive enthalpies of mixing, the atomic size mismatch and the relative elastic properties in these systems are quite different.

2. Computational methods

The simulations were performed using dilute Cu alloys as model systems, represented by embedded atom method type potentials [23] for Cu-Nb [24] and Cu-V [25] and a closely related angular dependent potential for Cu-Ta [26]. Table 1 lists properties of the alloy systems derived from these potentials. The MD code LAMMPS [27] and visualization using OVITO [28] were employed to run these simulations and help analyze the results. The samples in this study were created by two methods. For the first, a single spherical precipitate was introduced into the Cu matrix, selecting an arbitrary, low symmetry orientation. The cell was then relaxed by simulated annealing at 600 K at a hydrostatic pressure of 1 kbar for 100 psec, before bringing it to a temperature of 300 K at a pressure of 0 Pa. The annealing procedure was repeated 10 times to ensure stabilization. This procedure conserves precipitate shape while promoting interface relaxation. We note that at 600 K, diffusion is negligible, and thus the systems could stabilize during the short-term anneals without significant solute redistribution. In the second case, solute atoms were placed on randomly selected lattice sites in the Cu matrix and then relaxed by a similar annealing procedure. The two systems were then sheared cyclically using biaxial compression along the $\langle 100 \rangle$ (x,y,z) directions of the Cu matrix. In each cycle the sample was deformed to an engineering strain of 0.1 first in both the x and y directions, followed by similar strains in the y-z and z-x directions. This leads to an applied biaxial strain of 0.2 strain per compression and a total strain of 0.6 per cycle. All results are reported in terms of biaxial strain, ε, calculated using the trace of the imposed engineering strain tensor, which for biaxial compression is equal to the equivalent von Mises strain when neglecting elastic strains and small shape changes (see further details below). During the bi-axial compression, the third axis is maintained at zero stress leading to its subsequent elongation during the strain step. Thus following a full cycle, shape is nearly conserved and the system returns close to its initial dimensions. Since the strain is not completely isotropic, changes in the elongation along the free direction may lead to small changes in shape. Prior to each compression cycle, therefore, strain rates were modified by up to 2% per orientation, relative to the nominal value, in order to preserve the shape of the computational cell at the end of each cycle. Simulations were performed using strain rates between 1×10^8 s^{-1} and 5×10^9 s^{-1}, with no significant difference in the resulting steady states, but this will be discussed in more detail below. This insensitivity to strain rate indicates that there are no significant thermal contributions to the observed kinetics, although these are expected to be small in any case during deformation at 300 K. Results were also insensitive to changes in the total strain accumulated per compression, at least between 0.15 and 0.25. This is consistent with the fact that elastic strains per step are very small, accounting for less than 1% of the imposed strain. For strains less than 0.1 per step, elastic strains become more noticeable, especially in the initial stages of the simulations, reaching $\approx$10% of the imposed strain, and leading to results that are sensitive to the strain per step. System sizes were varied between 10^5 and 10^8 atoms, depending on the alloy concentration. We verified that there were no significant effects of size on the steady state configurations, as characterized by the phase composition, energy and chemical order, although some qualification of this point will be presented in section 4. Systems were simulated until steady states were attained; this required total accumulated bi-axial strains of up to ~600 in some cases. It is noteworthy that strains of the order of 100's $-$1000's are available experimentally using techniques such as ball-milling and HPT, and sometimes these high strains are required to achieve steady state. The strain required for steady state, however, depends on the length scale of the relevant microstructural features. Since our computational cell is quite small, the strain required for steady state tends also to be small. The small size, however, limits the materials problems we can investigate, as we will illustrate in the discussion section.

Structural identification of atoms was performed using the centro-symmetry parameter, which assigns low values to atoms with high crystalline symmetry [42]. Atoms within the amorphous phase where identified as those that have an average centro-symmetry parameter higher than 8, which was taken as an average over the atom in question and its 12 nearest neighbors. While centro-symmetry parameter is highly efficient in determining if an atom is located at a crystalline site, the local averaging ensured that only atoms embedded in non-crystalline environment were identified as amorphous, thus minimizing the counting of point defects.

3. Results

3.1. Dynamics of phase evolution during severe plastic deformation

We begin by providing an overview of the range of shear mixing behaviors in highly immiscible alloys for three specific alloys, $Cu_{94}Nb_6$, $Cu_{94}V_6$, and $Cu_{86}Ta_{14}$. The initial conditions for these simulation events was a spherical BCC precipitate embedded in a FCC Cu matrix. Deformation begins with dislocations gliding in the Cu matrix, with no dislocations observed cutting through the precipitate, and virtually no co-deformation of the BCC particle taking place. This is seen in Fig. 1(a–c) where a snapshot of the dislocation

Table 1
Properties of solutes derived from EAM potentials. Heat of mixing (H_0) and atomic volume (V_0) provided at infinite dilution in FCC Copper. Atomic volume of copper is 11.81 Å^3. Subscripts c and a refer to crystalline and amorphous states.

	G_{Cu}(GPa)	G_c(5%) (GPa)	G_a(10%) (GPa)	V_0(Å^3/atom)	H_0(eV/atom)
Cu-Nb [24]	72	30	5	17.9	1.3
Cu-V [25]	72	25	17	14.0	0.75
Cu-Ta [26]	76	30	19	18.0	1.6

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