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Martensitic transformation to monoclinic phase in bulk B2–CuZr

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ABSTRACT

Shape memory alloys, like B2–CuZr, are a class of materials that have the ability to recover their original shape when subjected to specific thermomechanical conditions. In this work, we carry out molecular dynamics simulations of bulk B2–CuZr to study its martensitic transformation at atomic level. For this purpose, uniaxial tensile tests are performed at temperatures ranging from 1 K to 600 K. We show that all cases exhibit pseudoelasticity by undergoing phase transition from B2 to monoclinic phase along the {110} planes, instead to an R phase as reported in previous works. We obtain the Bain path employing two different interatomic potentials. One potential exhibits martensitic transformation from B2 to monoclinic to body–centered tetragonal structure, while using the other potential a transition from B2 to monoclinic structure is observed, being absent the body–centered tetragonal phase. Reversibility of this transformation is confirmed by performing uniaxial tensile/compressive tests. Finally, a stress–temperature phase diagram is presented as a tool to estimate the stress required to initiate martensitic transformation of bulk B2–CuZr phases.

1. Introduction

Martensitic transformation (MT) is a mechanism which appears in different engineering functional materials, such as strengthened steel, polymers and shape memory alloys (SMAs). An outstanding property of MT is its reversibility to go from one phase to another under certain thermomechanical or magnetic conditions. Thus, SMAs have been employed in many engineering fields, such as structures and composites [1], automotive [2], aerospace [3] and micro-electromechanical systems (MEMS) [4]. Among the different SMAs available in the industry, of our interest is the case of the B2–CuZr alloy due to its application in metallic glasses (MG). It is widely known that MGs posses high yield strength and hardness, but suffer from poor ductility and brittle fracture, which limit their applications. To overcome this difficulty, it has been proposed to manufacture shape memory metallic glass composites. The main concept is to integrate a SMA as a crystalline phase in bulk MG to produce transformation induced plasticity [5,6]. In the case of CuZr–based MGs, experimental results have reported that mechanical properties are enhanced when high volume fractions of the B2 crystalline phase, for instance 40–80%, are found in the system. It has also been observed that the stress–strain curve of the MG exhibits more than one yield point due to the MT and that plastic flow is stabilized with high concentrations of the crystalline phase, improving the ductility of the MG [7–9]. Regarding theoretical studies, it is important to remark that there exists a lack of works about the B2–CuZr system at the atomic level to further discuss this MT, since most of the available literature concentrates solely in the structural and mechanical properties of CuZr MGs [10–14] without the presence of any crystalline phase.

Molecular dynamics (MD) simulations have been performed in recent years to study the B2–CuZr system and its MT in order to give an atomic level description. Sutrakar et al. [15,16] carried out tensile tests of B2–CuZr nanowires. He reported that these nanowires exhibited a MT from an initial B2 phase to a final BCT phase via nucleation and propagation of {100} planes, where an intermediate R phase was observed. These findings were also supported by Cheng et al. [17] and Sopu et al. [18]. In addition, Cheng et al. stated that the BCT phase was a metastable one, which was later discussed by Sutrakar et al. [19], concluding that this phase is unstable. However, none of these authors observed a B2 to monoclinic transformation, which has been largely reported in experimental results [7,9,20]. Moreover, these authors employed only the first version of the interatomic potential for the CuZr alloy developed by Mendelev et al. [21], which overestimates the Cu–Zr interaction. This drawback, among others, was overcome in a new version of the CuZr potential [22], where new data from experimental and first principles calculations were introduced to improve the accuracy of the semi–empirical potential. Thus, it is important to revisit the phase transformation of B2–CuZr samples using both potentials.

Thus, in order to get a better insight of B2–CuZr phase transformation, at an atomic level, some fundamental questions about its martensitic transformation should be addressed, for instance, what are

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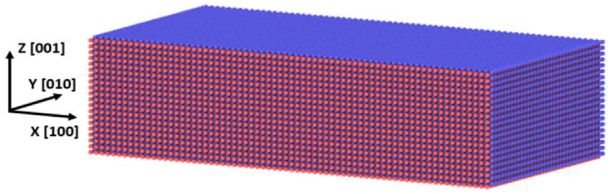

Fig. 1. Bulk B2–CuZr with periodic boundary conditions.

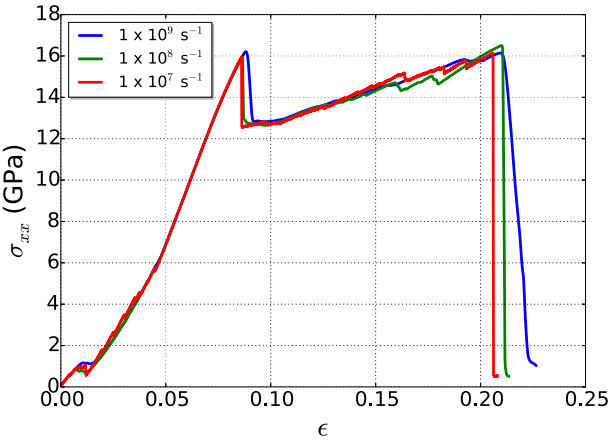

Fig. 2. Uniaxial tensile test of bulk B2–CuZr at 1 K and different strain rates.

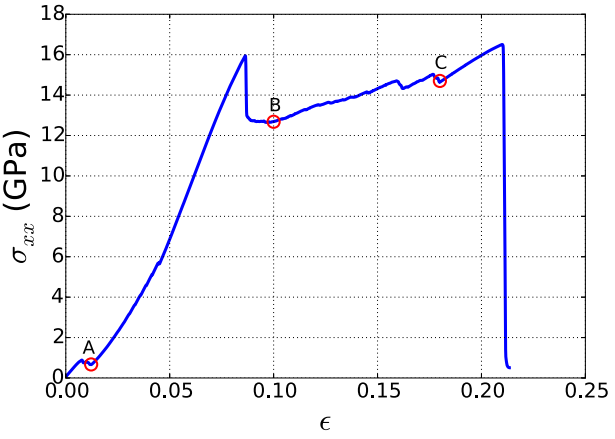

Fig. 3. Stress–strain curve for bulk B2–CuZr at 1 K and at 10^8 s^{-1} strain rate.

the structures of B2–CuZr along the transformation?, is the final structure stable?, what are the transformation paths? and finally, under what thermomechanical parameters the transformation takes place? The main goal of this work is to provide an answer to these questions.

In this work, we carry out MD simulations of bulk B2–CuZr under uniaxial tensile loading considering different temperatures, ranging from 1 K to 600 K, as well as different strain rates. Bulk systems have been selected over nanowires in order to neglect surface effects and to ease structural and phase transformation analysis. Also, the Bain path is calculated using both interatomic potentials developed by Mendelev et al. [21,22], in order to elucidate the differences in the MT. Reversibility of the transformation is checked and a stress–temperature phase diagram is obtained. This paper is organized as follows: in Section 2 we explain the simulation procedure and the tools for analysis used, in section 3 we present and discuss our results, and in Section 4 we draw the conclusions.

2. Simulation details

The B2–CuZr system under study has dimensions of 226.8 × 113.4 × 64.8 Å^3, with a lattice parameter of 3.24 Å and containing 98000 atoms, as shown in Fig. 1, where Cu and Zr atoms are colored blue and red, respectively. Periodic boundary conditions are imposed in all directions. To perform molecular dynamics simulations, it is necessary to adopt an adequate interatomic potential. In this work we employ the embedded-atom method (EAM) potential proposed by Mendelev et al. [22] for the CuZr system. The EAM gives the total energy of an atomic system in the form

$$E_i = F_\alpha\left(\sum_{j\neq i}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{j\neq i}\varphi_{\alpha\beta}(r_{ij}), \tag{1}$$

where F is the embedding energy which is a function of the atomic electron density ρ. In the second term, φ is a pair potential interaction and α and β are the element types of atoms i and j.

In order to carry out uniaxial tensile tests in bulk B2–CuZr, the molecular dynamics code LAMMPS developed by Plimpton et al. [23] is used. The procedure of the simulations is the following. Firstly, the energy of the system is minimized using the conjugate gradient method. Secondly, the Langevin thermostat at a constant temperature T and the Berendsen barostat at zero pressure are applied for 100 ps, using 1 fs as the integration time step. T is the target temperature to be studied, ranging from 1 K to 600 K. After these two steps, the sample is loaded along the [100] direction. Three different strain rates are considered, namely, 10^7 s^{-1}, 10^8 s^{-1} and 10^9 s^{-1}. The strain is applied on the system by rescaling the positions of atoms each time step. The temperature is kept constant at T using the Langevin thermostat. In order to analyze our simulation, we use several diagnostic tools. For stress–strain curve, we evaluate the σ_{xx} component of the stress tensor, as well as the axial component of the strain tensor, denoted as ε. The analysis of the atomic structure is made by means of the pair distribution function, the common neighbor analysis (CNA) [24,25] and the local atomic shear strain η^{Mises} [26]. This parameter requires two atomic configurations, the current and the reference one. The first step is to seek a local affine transformation $\mathbf{J}_i$ that best map

$$\{\mathbf{d}^0_{ji}\} \rightarrow \{\mathbf{d}_{ji}\},\ \forall\, j \in N^0_i, \tag{2}$$

where $\mathbf{d}$ are vector separations between atom i and each neighbor j. Here the superscript 0 stands for reference configuration, and N^0_i is the number of neighbors of atom i at the reference configuration. Then, we seek $\mathbf{J}_i$ that minimizes

$$\sum_{j\in N^0_i}\left|\mathbf{d}^0_{ji}\mathbf{J}_i - \mathbf{d}_{ji}\right|^2 \rightarrow \mathbf{J}_i = \left(\sum_{j\in N^0_i}\mathbf{d}^{0T}_{ji}\mathbf{d}^0_{ji}\right)^{-1}\left(\sum_{j\in N^0_i}\mathbf{d}^{0T}_{ji}\mathbf{d}_{ji}\right). \tag{3}$$

With $\mathbf{J}_i$, the Lagrangian strain matrix can be calculated as

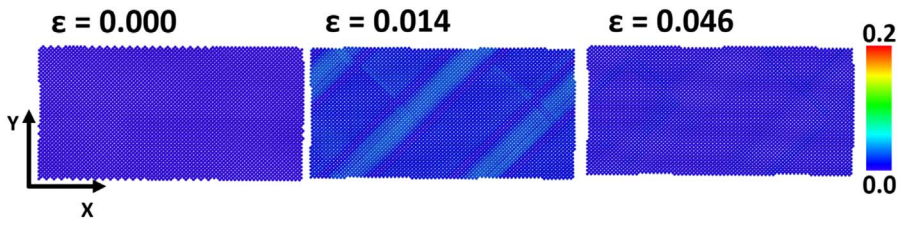

Fig. 4. Bulk B2–CuZr at different strains. Atoms are colored according to the local atomic shear strain. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)