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Cold welding of copper nanowires with single-crystalline and twinned structures: A comparison study

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HIGHLIGHTS

- Cold welding processes of copper nanowires were explored by molecular simulations.
- Twinned nanowires can be successfully welded through small loadings.
- Welding processes were compared between single-crystalline and twinned nanowires.

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ABSTRACT

In this article, molecular simulations were adopted to explore the cold welding processes of copper nanowires with both single-crystalline and fivefold twinned structures. It was verified that the twinned nanowires exhibited enhanced strength but lowered elastic limit and ductility. Both nanowires could be successfully welded through rather small loadings, although their stress–strain responses toward compression were different. Meanwhile, more stress was accumulated in the twinned nanowire due to repulsive force of the twin boundaries against the nucleation and motions of dislocations. Moreover, by characterizing the structure evolutions in the welding process, it can be ascertained that perfect atomic order was finally built at the weld region in both nanowires. This comparison study will be of great importance to future mechanical processing of metallic nanowires.

1. Introduction

In the rapidly developing field of nanotechnology, welding technique plays an important role in the architecture of nanodevices and thus has attracted extensive attention [1–5]. In recent years, joining has been successfully realized among many low-dimensional nanostructures by direct heating [1], focused electron beam, laser radiation [2], or inducing voltage (electricity) [3–5]. In these most widely adopted approaches, local temperature rising or even melting is inevitably brought. Therefore, the relevant process not only requires precise control of the heat, but may also result in irreversible damage of the materials and consequently permanent loss of function. In contrast, welding without involvement of heating, that is, cold welding, avoids these disadvantages and hence has irreplaceable superiority. Actually, research on cold welding has been reported since decades ago [6]. However, its application was generally limited in macroscopic materials, and relatively large external loads were normally demanded. This situation has been changed since a breakthrough progress was achieved by Whitesides and coworkers who interconnected gold films through cold welding by very low loads under ambient conditions [7]. At present, cold welding between thin films have been frequently employed in modern manufacturing of microelectronic and photoelectric devices [8–12]. Naturally, it raises the question of whether cold welding can be implemented in low-dimensional nanostructures such as nanowires (NWs) and nanoparticles (NPs), which are the indispensable building blocks in microelectromechanical systems (MEMS) and are of great significance in material science [13–15].

Relevant experiments have been accomplished by Lou and coworkers, who have joined two Au single-crystalline NWs through mechanical contact under relatively low applied pressure at room temperature [16]. High-resolution transmission electron microscopy and in situ measurements revealed that the welds were of high quality, which was attributed to the nanoscale sample dimensions, oriented-attachment mechanisms and mechanically assisted fast surface-atom diffusion. This achievement is of great significance to the bottom-up fabrication of nanodevices.

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Although cold welding of different systems has been extensively investigated [16–18], there are still some pending problems that need to be clarified. For example, to the best of our knowledge, its adaptability in twinned NWs remains unclear. As is known, experimental explorations have demonstrated that introducing twin boundary into metals can be used as an approach to significantly enhance their mechanical strength and at the same time to retain their high electrical conductivity [19]. Therefore, metallic NWs with twinned structures are considered to have broad potential applications in microcircuits. Based on this consideration, in this article we performed molecular dynamics (MD) investigations on the cold welding processes of copper NWs with both single-crystalline and twinned structures to make a comparison study. Since it is rather difficult or even impossible to experimentally capture the atomistic structure evolution of nanomaterials under continuous loading, this exploration can remedy the deficiency of experiments to a certain extent and provide an atomic-level insight for the forthcoming experiments. The article is organized as follows. A brief description of the simulation methodology is given in Section 2. The calculated results and discussion are presented in the third section. The main conclusions are summarized in the fourth section.

2. Simulation methodology

Two types of Cu NWs with axes along the [110] orientation, namely single-crystalline nanowire (SCNW) with close circle cross-section and fivefold twinned nanowire (FTNW) with pentagonal geometry, were constructed from a large face-centered cubic (*fcc*) single crystal of copper, as illustrated schematically in Fig. 1. Total numbers of atoms in the two types of NWs were chosen to ensure that they possessed the same length (26.4 nm) and diameter (3.3 nm). In order to simulate the mechanical control of the movement in experiments, six atomic planes at both ends of each NW were fixed.

Based on our previous works [20–23], the quantum corrected Sutton–Chen (Q–SC) type potentials were adopted to describe the interatomic interactions [24]. These potentials represent many-body interactions, and their parameters were optimized according to the lattice parameter, cohesive energy, bulk modulus, elastic constants, phonon dispersion, vacancy formation energy, and surface energy, resulting in an accurate description of many properties of metals and their alloys [25–27]. The total potential energy for a system of atoms can be expressed as

$$U = \sum_i U_i = \sum_i \varepsilon \left[\frac{1}{2} \sum_{j \neq i} V(R_{ij}) - c\sqrt{\rho_i} \right] \tag{1}$$

in which $V(R_{ij})$ is a pair interaction function defined by the following equation

$$V(R_{ij}) = \left(\frac{a}{R_{ij}} \right)^n \tag{2}$$

accounting for the repulsion between the i and j atomic cores; ρ_i is a local electron density accounting for cohesion associated with atom i defined by

$$\rho_i = \sum_{j \neq i} \left(\frac{a}{R_{ij}} \right)^m \tag{3}$$

In Eqs. (1)–(3), R_{ij} is the distance between the ith and the jth atoms; a is a length parameter scaling all spacings; c is a dimensionless parameter scaling the attractive terms; ε sets the overall energy scale; n and m are integer parameters. The model parameters for Cu are given as follows: $n = 10$, $m = 5$, $\varepsilon = 5.7921 meV$, $c = 84.843$, and $a = 3.6030$Å [24].

Upon starting molecular dynamics simulations, both NWs were first quasi-statically relaxed to a local minimum energy state through the conjugate gradients method [28]. After full relaxation, they were subjected to a continuous unaxial loading process, which was applied along the length direction with a strain of 0.25% as the increment step. Note that the positive strain makes the frozen atomic planes at both ends of the NW move away from each other and leads to the stretching of the NW until it breaks, which produces two tips for the subsequent welding. In contrary, the negative strain results in the compression of the NW, which simulates the welding process. At each loading step, MD simulations were carried out at room temperature of 300 K and for relaxation time of 200 ps to reach the equilibrium state, during which atomic coordinates, velocities and energies were recorded. The desired temperature was maintained by Nose-Hoover thermostat [29], and the equations of atomic motion were integrated by the Verlet-velocity algorithm [30] with a 1 *fs* time step.

In the loading process, the local stress σ_n at the i_{th} atom site can be written as

$$\sigma_n = \frac{1}{3} \sum_{\alpha=1}^{3} \sigma_{\alpha\alpha} = \frac{1}{3} \sum_{\alpha=1}^{3} \left(\frac{1}{2\Omega_i} \sum_{j \neq i} F_{ij}^{\alpha} R_{ij}^{\alpha} \right) \tag{4}$$

where F_{ij} and R_{ij} are the force and distance between atoms i and j. Ω_i is the local volume between atom i and all its neighbor atoms [31].

3. Results and discussion

In order to obtain the tips for the later cold welding, both NWs were subjected to continuous stretching until their breakings. Their stress–strain responses are presented in Fig. 2.

As is seen, the NWs firstly experience a short elastic deformation, indicated by the linear region in the curves. Afterwards, they entered into the stage of plastic deformation until fracture. It can be found from the figure that the yielding stresses are 3.83 and 5.25 GPa respectively for the SCNW and FTNW. Meanwhile, their fracture strains are respectively 59.5% and 19.5%. The significantly smaller fracture strain of the FTNW could also be verified by comparing the final lengths of the two NWs in the inset snapshots.

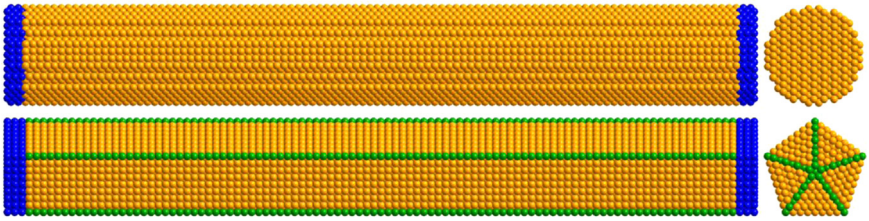

Fig. 1. Schematic illustration of Cu SCNW (above) and FTNW (below) and their corresponding cross sections. Blue spheres denote the fixed atoms, and green spheres denote the atoms located at twin boundaries. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)