International Journal of Plasticity 87 (2016) 100–113

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Atomistic study of fundamental character and motion of dislocations in intermetallic Al_2Cu

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ARTICLE INFO

Article history:
Received 28 July 2016
Received in revised form 4 September 2016
Available online 22 September 2016

Keywords:
A. Dislocations
B. Crystal plasticity
B. Metallic material
Molecular dynamics simulation

ABSTRACT

Atomic scale study of the character and motion of dislocations in Al_2Cu will provide insights into understanding the superior mechanical properties of Al–Al_2Cu alloys. Using atomistic simulations, we studied seven potential slip systems $(110)\langle 001\rangle$, $(010)\langle 001\rangle$, $(310)\langle 001\rangle$, $(010)\langle 100\rangle$, $(110)\langle 1\bar{1}0\rangle$, $(110)\frac{1}{2}\langle 1\bar{1}1\rangle$ and $(112)\frac{1}{2}\langle \bar{1}\bar{1}1\rangle$ in Al_2Cu with body centered tetragonal structure. We found that three edge dislocations with Burgers vector $\langle 001\rangle$ on glide planes (110), (010), and (310), show an extended core and are predicted to be glissile at room and moderate temperatures. Other four edge dislocations associated with slip systems $(010)\langle 100\rangle$, $(110)\langle 1\bar{1}0\rangle$, $(110)\frac{1}{2}\langle 1\bar{1}1\rangle$ and $(112)\frac{1}{2}\langle \bar{1}\bar{1}1\rangle$ and three screw dislocations with Burgers vectors $\langle 001\rangle$, $\langle 110\rangle$, and $\frac{1}{2}\langle \bar{1}\bar{1}1\rangle$ show a condensed core, and exhibit significantly higher Peierls barrier for glide at room temperature. Furthermore, the interaction of dislocation dipole associated with slip system $(110)\langle 001\rangle$ results in the climb of the extended-core dislocation at room temperature through three stages: the extended core condenses, the leading partial dislocation climbs accompanying the creation of vacancies (resulting in a non-planar core), and the two partials with non-planar core collectively glide on the neighboring slip planes associated with atomic shuffles.

1. Introduction

Metal-intermetallic eutectic composites are potential candidates for structural applications at ambient and elevated temperatures (Umakshi, 1993). Al-based alloys, such as Al–Cu (Park et al., 2009, 2010; Yanilkin et al., 2014; Csontos and Starke, 2005; Prados et al., 2013; Bonnet and Loubradou, 2002; Liu, 2011), Al–Mg (Youssef et al., 2006; Jobba et al., 2015; Zhou et al., 2003; Hales and McNelley, 1988), Al–Ni (Muñoz-Morris et al., 2009; Rajan et al., 2008; Shield, 1995), Al–Si (Mabuchi and Higashi, 2001; Nogita et al., 2006; Picu et al., 2011), etc. have attracted the most attention because of their

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http://dx.doi.org/10.1016/j.ijplas.2016.09.005
0749-6419/

lightweight, four times lower density as compared to steel (Umakshi, 1993). Most of the reported Al-based state-of-the-art commercial alloys are precipitation or dispersion hardened. For Al–Cu alloys, Al_2Cu precipitates are formed in plate-like structures (Park et al., 2009, 2010; Yanilkin et al., 2014; Csontos and Starke, 2005; Prados et al., 2013; Bonnet and Loubradou, 2002; Liu, 2011; Russell and Ashby, 1970). These precipitates developed several well-defined orientation relationships (ORs) with matrix Al (Gao et al., 2014; Howe et al., 1995; Ignat et al., 1978; Knowles and Stobbs, 1988). Under mechanical loading at room temperature, Al_2Cu precipitates in these composites elastically deform due to the brittle nature of Al_2Cu phases (high friction force associated with dislocations motion), acting as strong obstacles for dislocation motion (Prados et al., 2013; Han et al., 2004; Bonnet, 2002). When precipitates and matrix geometrically co-deform under mechanical loading, Al_2Cu precipitates may be subjected to higher stresses than matrix Al due to its higher elastic modulus than Al. They elastically deform without apparent plasticity at room temperature, and often failure due to cracks (Chadwick, 1963; Chanda and Murty, 1992; Khan and Liu, 2012). At elevated temperatures (>300 °C), Al_2Cu precipitates can plastically deform via dislocations (Chadwick, 1963; Chanda and Murty, 1992; Khan and Liu, 2012). Dislocations in intermetallic phases are preferably nucleated from phase boundaries because of interface ledges/steps and slip transmission for dislocations from matrix into Al_2Cu precipitates (Bonnet, 2002; Li and Wawner, 1998; Nie and Muddle, 2000).

In order to enhance ductility and strength at room temperature, the current focus is on producing Al–Cu alloys with a high volume fraction of intermetallic reinforcement (in other words, reduction in interphase spacing or interlamellar spacing for regular eutectic) with the help of either rapid solidification with alloying additions (Park et al., 2009, 2010; Shield, 1995; Witkin et al., 2003; Otsuka and Shimizu, 1970; Trivedi et al., 2004) or severe plastic deformation (SPD) techniques (Prados et al., 2013; Murayama et al., 2001; Loucif et al., 2010; Tao et al., 2013; Pérez-Prado and Ruano, 2004; Valiev et al., 2000). For example, Al–Cu–Si alloys containing a bimodal distribution of eutectic colonies exhibit a high strength and a compressive plastic strain of 2% at room temperature (Park et al., 2009, 2010). Severe plastic deformation techniques, such as equal channel angular pressing (Prados et al., 2013; Murayama et al., 2001), high pressure torsion (Loucif et al., 2010; Tao et al., 2013), and accumulated rolling (Pérez-Prado and Ruano, 2004; Valiev et al., 2000), have been demonstrated to produce the bulk nanostructured metals with a grain size or layer thickness in nanometer or sub-micrometer ranges (Pérez-Prado and Ruano, 2004; Valiev et al., 2000; Zeng et al., 2013; Uenishi et al., 1991), accompanied with a high density of dislocations stored in intermetallic phase. *In situ* straining experiments of Al_2Cu–Al composites in a transmission electron microscope (TEM) have shown dislocations bypassing through Al_2Cu plate-shaped particles by shear at multiple locations along the interphase boundaries, and the formation of a complex configuration of lattice dislocations pinned at both ends on a particle interface (Liu, 2011; Russell and Ashby, 1970). In addition, SPD also leads to the formation of non-equilibrium solid solutions (Uenishi et al., 1991; Yang et al., 2013), disordering (Korznikov et al., 1999) or amorphization (Inoue, 1998; Eckert et al., 1991) in intermetallic phase. The decomposition or instability of intermetallic phase during heavy plastic deformation has been partially ascribed to dislocations and defected interfaces created during straining (Umakshi, 1993). Dislocations have been demonstrated to provide rapid diffusion channels and adiabatic heating of the samples during plastic deformation (Hirth and Lothe, 1982; Schroll et al., 1998). Dislocations crossing the precipitates may drag the interstitial or vacancy atoms with them out of the precipitate (Gridnev and Gavrilyuk, 1982). In addition, it has been observed in experiments that dislocation climb occurs in intermetallic phase associated with the change in dislocation core structures (Umakshi, 1993; Appel, 2001; Anton et al., 1989). Moreover, creation of slip steps at the interphase boundaries of the precipitate may lead to their thermodynamic instability. Nevertheless, dislocations and their motion and reactions are presumed to be responsible for the structural instability of intermetallic phase.

The possible dislocation types in Al_2Cu (θ) are directly related to its C16 body centered tetragonal structure. An unit cell contains 12 atoms with internal coordinates of Cu: {0,0,1/4}; {0,0,3/4}; {1/2,1/2,1/4}; {1/2,1/2,3/4}; and Al: {0.1541, 0.6541, 0}; {0.3459, 0.1541, 0}; {0.8459, 0.3459, 0}; {0.6541, 0.8459, 0}; {0.8459, 0.6541, 0.5}; {0.6541, 0.1541, 0.5}; {0.1541, 0.3459, 0.5}; {0.3459, 0.8459, 0.5}. The most complete families of glide planes deduced from the close packed planes according to the crystallography of C16 body centered tetragonal structure are {110}, {100}, {011}, and {112}; the major slip systems include $\{110\}\langle 001\rangle$, $\{110\}1/2\langle 111\rangle$, $\{200\}\langle 001\rangle$, and $\{112\}1/2\langle 111\rangle$ (Ignat and Durand, 1976). Dislocations with Burgers vector [110] have been identified along grain boundaries using high resolution TEM (Bonnet, 2002; Bonnet and Loubradou, 2002). But it was not clear whether such dislocations could glide in Al_2Cu (θ) because the Burgers vector is too large (Bonnet and Loubradou, 2002; Chanda and Murty, 1992). In addition, a quite unusual core splitting has been observed for $(110)1/2\langle 111\rangle$ on the (110) plane, and large planar faults have been noticed on (001) (Bonnet and Loubradou, 2002; Knowles and Stobbs, 1988). In summary, Al_2Cu (θ) is brittle at lower temperatures, but plastically deformable via dislocation glide and climb at high temperatures. The brittle-ductile (BD) transition for Al_2Cu (θ) phase in Al–Al_2Cu (θ) composites occurs at 300 °C (Ignat et al., 1978), and at 375 °C in Al_2Cu (θ) single crystals and polycrystals by compression testing (Chanda and Murty, 1992), indicating the drop of the BD transition temperature of Al_2Cu (θ) in composites. With decreasing the interphase spacing and the thickness of intermetallic phase in metallic-intermetallic composites, the interaction force among dislocations accumulated on the adjacent phase boundaries will increases and may favor slip transmission and dislocation glide in intermetallic phase (Salehinia et al., 2014; Wang and Misra, 2014; Embury and Hirth, 1994). As demonstrated in Al–TiN system, room temperature plasticity is achievable (Li et al., 2014). However, plasticity in Al_2Cu lamellae at room temperature, more precisely, characteristics of dislocations, has been rarely studied at atomic scale (Chen and Ma, 2013).

In this paper, we employed molecular dynamics/statics (MD/MS) simulations with empirical interatomic potentials (Apostol and Mishin, 2011) to study characteristics of dislocations associated with slip systems $(110)\langle 001\rangle$, $(010)\langle 001\rangle$, $(310)\langle 001\rangle$, $(010)\langle 100\rangle$, $(110)\langle 1-10\rangle$, $(110)\frac{1}{2}\langle 1\bar{1}1\rangle$ and $(112)\frac{1}{2}\langle\bar{1}\bar{1}1\rangle$. Furthermore, we investigated interaction of dislocation