International Journal of Solids and Structures 51 (2014) 1149–1163

Contents lists available at ScienceDirect

International Journal of Solids and Structures

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

Interaction between edge dislocations and amorphous interphase in carbon nanotubes reinforced metal matrix nanocomposites incorporating interface effect

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ARTICLE INFO

Article history:
Received 27 June 2013
Received in revised form 2 December 2013
Available online 13 December 2013

Keywords:
Amorphous interphase
Edge dislocations
Image force
Carbon nanotube

ABSTRACT

Dislocations mobility and stability in the carbon nanotubes (CNTs)-reinforced metal matrix nanocomposites (MMNCs) can significantly affect the mechanical properties of the composites. However, current processing techniques often lead to the formation of coated CNT (amorphous interphase exists between the reinforcement and metal matrix), which have large impact upon the image force exerting on dislocations. Even though the importance of the interphase zone formed in metal matrix composites has been demonstrated by many studies for elastic properties, the influence of interphase on the local elastoplastic behavior of CNT-reinforced MMNCs is still an open issue. This paper puts forward a three-phase composite cylinder model with new boundary conditions. In this model, the interaction between edge dislocations and a coated CNT incorporating interface effect is investigated. The explicit expressions for the stress fields and the image force acting on an edge dislocation are proposed. In addition, plastic flow occurring around the coated reinforcement is addressed. The influences of interface condition and the material properties of coated CNT on the glide/climb force are clearly analyzed. The results indicate that the interface effect becomes remarkable when the radius of the coated reinforcement is below 10 nm. In addition, different from the traditional particles, the coated CNT attracts the adjacent edge dislocations, causing pronounced local hardening at the interface between the interphase and the metal matrix under certain conditions. It is concluded that the presence of the interphase can have a profound effect on the local stress field in CNT-reinforced MMNCs. Finally, the condition of the dislocations stability and the equilibrium numbers of dislocations at a given size grain are evaluated for considering the interface effect.

1. Introduction

Carbon nanotubes (CNTs) have attracted tremendous expectation as reinforcements to improve the mechanical performance of monolithic materials due to their extraordinary mechanical properties as compared with pure metal (Treacy et al., 1996). Numerous research studies have been undertaken on synthesis and characterization of CNT/metal matrix composites since the first article appeared in 1998 on CNT/Al composite (Kuzumaki et al., 1998). Recently, Bakshi et al. (2010) have presented a review summarizing the research work carried out in the field of carbon nanotubes reinforced metal matrix nanocomposites (MMNCs), which elucidated the influence of CNT volume concentration, dispersion, strengthening mechanisms, and CNT-matrix interfacial conditions on the overall elastic and plastic behavior of the composites.

However, compared with CNT-reinforced polymer matrix composites (PMCs) (Fisher et al., 2003; Odegard et al., 2003; Odegard et al., 2004; Coleman et al., 2006; Namilae and Chandra, 2006; Wang et al., 2008; Jia et al., 2011; Tehrani et al., 2011) and ceramic matrix composites (CMCs) (Flahaut et al., 2000; Rul et al., 2004; Xia et al., 2004; Yamamoto et al., 2008; Ahmad et al., 2010; Liu et al., 2011a), studies on MMNCs reinforced by CNT are comparatively fewer, and the improvement of the mechanical properties of bulk CNT/metal matrix composites is not commensurate with the expectation. This is mainly because of difficulties in uniformly distributing CNT in most metallic matrices and weak interfacial issues between the reinforcements and matrices. Agglomeration of CNT could lead to premature failure of the composites, and various processing techniques have been adopted to avoid such a highly undesirable condition. In addition, the interfaces between CNT

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http://dx.doi.org/10.1016/j.ijsolstr.2013.12.011

and metal matrix are also critical to the pursuit of enhanced mechanical properties of the composites, even when CNT are uniformly dispersed. The most possible phenomenon may be the formation of nanosize carbides on the interfaces between CNT and matrix and this may affect the load transfer condition between them (Ci et al., 2006; Deng et al., 2007; Esawi et al., 2010). These particles are likely to be the by-products of chemical reactions between the metal powders and amorphous carbon atoms around pristine CNT and found to be closely attached to the surfaces of the reinforcement. Moreover, Kim et al. (2008) have observed many oxygen-rich regions existing near the CNT or on their surfaces. The good agreement of yield strength and elastic modulus between the measured values and the ones calculated by both the shear-lag and the Eshelby model, demonstrating that oxygen atoms presenting at the CNT/Cu interface play a significant role in accommodating the load transfer between matrix and reinforcement. Besides, the amorphous interphase was revealed to form around CNT in CNT/Cu composites after hydrogen reduction and consolidation (Cho et al., 2012), which was composed of amorphous carbon atoms and oxygen atoms. Similarly, Balani and Agarwal (2008) also observed that the molten metal spread uniformly on the surfaces of CNT and formed thin layers (about 20–25 nm) without any cracks. In fiber-reinforced composites, coatings on fibers are widely employed to improve the bonding conditions between fibers and matrix (Hashin, 2002; Gao et al., 2008). A coating layer can control the delamination of the interface and inhibit cracks initiated external to the reinforcement from damaging the matrix. Recently, Yang et al. (2013) have proposed a nonlinear multiscale modeling approach to characterize the elastoplastic behavior of CNT-reinforced PMCs with considering the interphase. The study focused on the identification of local elastic and plastic behavior of the interphase region from the well known elastoplastic properties of the nanocomposites. In a word, the presence of interphase around CNT in CNT-reinforced MMNCs can significantly affect the local stress field distribution and greatly change the load transfer conditions between reinforcement and matrix. Even though the importance of the interphase zone has been demonstrated by many investigations for elastic properties (Shen and Li, 2003; Mogilevskaya and Crouch, 2004; Mogilevskaya et al., 2010), studies on the influence of interphase on the local elastoplastic behavior of CNT-reinforced MMNCs is still an open issue. We expected to look into the issue in this paper.

Up until now, three strengthening mechanisms have been developed to predict the yield strength of CNT-reinforced MMNCs, two among them, namely Orowan strengthening and thermal mismatch, containing the dislocation effect (George et al., 2005; Li et al., 2009). Dislocations are the carriers of plasticity in crystalline materials and their mobility and stability around inclusions in the matrix can affect the mechanical behaviors of composites. CNT-reinforced MMNCs are often prepared under severe conditions, such as high temperature and high pressure (Xu et al., 1999; Kwon et al., 2009). Residual stresses will build up during the cooling process due to the significant coefficient of thermal expansion (CTE) and the elastic-plastic properties mismatch between CNT and matrix. The stresses around the reinforcement are large enough to cause plastic deformation in the matrix, especially in the interface region, and then generate small defects such as a high density of dislocations in the vicinity of nanosized particles (Hiratani et al., 2003; Aghababaei and Joshi, 2013). Ashby (1966) proposed that the stress concentration around a particle in a second-phase particle/matrix system was relieved by the nucleation and movement of prismatic loops along a secondary slip system. When the magnitude of the local resolved shear stress exceeds a certain value, dislocation loops (the pairs of opposite-signed edge dislocations) will be nucleated at random sites along the slip planes and punched out into the matrix (Taya et al., 1991; Shibata et al., 1992; Lubarda, 2011). The ductility improvement of CNT/Mg composites was observed to be the result of the initiation of prismatic slip and the activation of the basal slip system, and one of the main hardening reasons of the composites was identified to be the formation of sessile forest dislocations (Goh et al., 2008). These studies have shed significant insights into the generation and movement of dislocations in CNT-reinforced MMNCs, but none has touched upon the interaction between dislocations and amorphous interphases encircled CNT. The interactions between dislocations and nearby second phase or misfit stress field are of great importance, which can modify the overall yield behavior of the composites (Qaissaunee and Santare, 1995; Hu et al., 2004; Khraishi et al., 2004; Wang et al., 2010). In view of this importance, the problem has received much attention in the last decades, and is often simulated by employing the three-phase composite cylinder model (Dundurs and Mura, 1964; Luo and Chen, 1991; Ru, 1999; Xiao and Chen, 2001; Sudak et al., 2002; Wang and Shen, 2002; Fang et al., 2009a; Wang and Pan, 2011). In addition, it is well known that in the classical dislocations-particles analysis, dislocations are repelled from second phase when the shear moduli of the inclusions are higher than those of the matrices. However, when interface bonding is modified by imperfect interface boundary conditions or diffusional relaxations, these interactions may be completely reverse (Gao, 1992).

In recent years, to deeply address the size-dependent elastic and plastic fields created by nanoscale inclusions, the surface/interface stress model has been extensively developed on account of the rapid development of nanotechnology (Fang and Liu, 2006; Lim et al., 2006; Zhang et al., 2010; Bakhshayesh et al., 2012; Gutkin et al., 2013). Jiang et al. (2006) has developed a cohesive law for CNT/polymer interfaces to estimate the surface effect by employing the atomistic model. Since atoms near and between the interfaces have different energies from those in the interior of the inclusions or matrix, surface/interface stress appears. In general, when the matrix with large grain size, the volume ratio of the interface region to the bulk material is small, the effect of the interface stress is insignificant. However, for fine-scaled materials, especially for nanocrystalline composites, with a large ratio of the interface region to the matrix, the interface plays a very important role in affecting the elastic-plastic deformation behaviors of the composites (Yassar et al., 2007). A lot of theories (Liu et al., 2009; Liu et al., 2010) give us some hints that the difference of the plastic deformation behavior between nanostructured materials and coarse-grained materials is essentially size-dependent. In the present study, we pay close attention to the impact of interface stress upon the mobility and stability of dislocations.

In addition to the role of interphase and interface, it is also important to consider the influence of the matrix grain size on the stresses experienced by dislocations and their stability. Compared with the coarse grains, the activity of conventional dislocation sources is inhibited in nanoscale grains. In that situation, amorphous intergranular boundaries (AIBs) are expected to become the sources for lattice dislocation nucleation in deformed nanocomposites (Bobylev et al., 2009). In addition, atomic simulations Wang et al. (2007) demonstrated that the amorphous crystalline interfaces (ACIs) exhibited unique inelastic shear transfer characteristics, different from those of grain boundaries (GBs). Dislocations can be emitted from ACIs or from GBs or ACIs-GBs intersections and absorbed at the opposite ACIs. However, if grain size is relatively small (of the order of nanometers), the dislocations emitted from ACIs usually be retarded at the opposite GBs and impede further dislocations emission, the ductility is often reduced dramatically. As a result, the addition of nanoscale amorphous layers may offer great benefits in constructing the plasticity of crystalline composites, and opening new approaches for improving their strength and ductility. However, the micromechanism of dislocations emitted from the interface between interphase and matrix is unclear. Such a