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A quantitative understanding on the mechanical behaviors of carbon nanotube reinforced nano/ultrafine-grained composites

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ABSTRACT

The mechanical responses of carbon nanotube (CNT) reinforced nano/ultrafine-grained metal matrix composites (MMCs) with the reinforcement located at grain boundaries and atomically disordered regions near the reinforcement have not been discussed yet. Here a theoretical model based on dislocation-controlling constitutive relations of metal matrix and strain gradient effect is adopted to quantitatively understand the contributions of strengthening mechanisms to the mechanical response of these composites. CNT-reinforced nano/ultrafine-grained MMCs will be treated as a two-phase composite with CNT-free regions surrounded by CNT-containing domains, whose mechanical behaviors are different from that of the matrix-only regions. The predictions of this model are in excellent agreement with available experimental results. During the process of deformation, geometrically necessary dislocations induced by strain gradient and thermal mismatch are limited within CNT-containing domains, and the thicknesses of these regions are obtained to be linearly proportional to matrix grain size by fitting with the experimental results. When the size of the reinforcement is large, the effect of thermal mismatch strengthening mechanism on the strength of MMCs is slight and can be ignored compared with the roles of Hall–Petch strengthening or load transfer effect.

1. Introduction

Carbon nanotube (CNT) has been expected as an ideal reinforcement in composites due to its special structure, high strength and stiffness along with low density [1–4]. Due to some technical difficulties in experiments, continuum modeling has been extensively applied to the analyses of CNT currently [5–7]. In addition, considerable work has been done to prepare CNT-reinforced metal matrix composites (MMCs) and characterize their elastic and plastic response [8], after the first article appeared on Al/CNT composites [9]. To predict the strength of MMCs, various strengthening mechanisms have been considered in a great deal of modeling methods [10,11]. These strengthening mechanisms typically contain grain refinement strengthening [12] (that is, Hall–Petch effect), thermal mismatch strengthening [13] due to the coefficient of thermal expansion (CTE) mismatch between second phases and metal matrix, Orowan strengthening [10] pronounced with reinforcement of low aspect ratio, load transfer behavior explaining the direct strengthening contribution from the existence of particulates and elastic mismatch strengthening [14]. It is necessary to develop theoretical models to quantitatively understand the determination of the combination of these potential strengthening mechanisms on the strength of CNT-reinforced MMCs, and a generally agreed upon theory has not been emerged yet [11].

Recently, Sanaty-Zadeh [15] has analyzed available current models for particulate-reinforced MMCs and performed comparisons between experiments to increase the precision of these models, in which the emphasis has been paid on the effect of Hall–Petch strengthening. In addition, a thorough analysis based on the results obtained from experimental observations and prediction models has been provided by Kim et al. [11]. Candidate strengthening mechanisms have been reviewed and various summation methods of these contributions have been summarized [11]. The attention of the aforementioned papers is mainly paid on particulate-reinforced MMCs, the load transfer effect is not obvious and a conclusion has been gained that grain refinement strengthening plays a significant role in yield strength of MMCs. However, these models do not taken into account the microstructure of matrix and location of the reinforcement. In addition, the distribution of matrix grain size is normally in micron range, while the addition of particulates into nano/ultrafine-grained metal matrix needs to be discussed in details because of the increasing studies of CNT-reinforced nano/ultrafine-grained MMCs [16,17].

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Experimental observations show that the distribution of CNT in MMCs exists certain random as a result of different preparing conditions and processing routes. All the reinforcement were observed to be located at grain boundaries (GBs) when CNT-reinforced Al matrix composites were produced by the combination of hot extrusion and spark plasma sintering [18]. In addition, transmission electron microscope (TEM) micrographs of GB layer of the sintered composites showed that the boundary layer between two grains consists of Al, CNT, amorphous carbon black and so on [18], which was obviously different from the microstructure of matrix grains. Kim et al. [19] observed from cross-sectional scanning electron microscopy (SEM) images of wet-etched 5 vol% CNT-reinforced Cu matrix composites that the interfacial regions near the reinforcement are chemically unstable and different from the Cu-only regions. In addition, atomically disordered regions closed to the reinforcement were also observed by high-resolution TEM [19]. Choi et al. [20] found that the work hardening capacity of CNT-reinforced nano/ultrafine-grained MMCs is not seem to be greatly affected by the content of the reinforcement, and attributed the phenomenon to the fact that CNT is mostly situated at GBs. Vogt et al. [21] observed that geometrically necessary dislocations (GNDs) induced by thermal mismatch are constrained to nanostructured interfacial layers in a bulk nano-grained MMC under different heat treatments and quenching conditions, and the absence of thermal mismatch strengthening on the strength improvement of the composites is presented. The location of CNT can affect the local microstructure of nano/ultrafine-grained MMCs, which is very critical for determining their overall mechanical behaviors [22]. In addition, the CNT-containing GB exhibits different deformation behaviors from that of nano/ultrafine-grained matrix and should be considered in theoretical models.

To obtain better combination of strength and ductility, composites are thought to be a breakthrough and CNT is introduced in nano/ultrafine-grained metal matrix [20]. Compared with coarse-grained ones, nanocrystalline materials have received much attention over the past decades because of outstanding physical and mechanical properties [23–25]. Besides the experimental studies, nanocrystalline solids have been widely investigated by a great deal of theoretical models [26]. For single phase nanocrystalline solids, researchers often treat them as composite materials consisting of grain interior (GI) and grain boundary affected zone (GBAZ) [27]. The grain size effect is thought to originate from the presence of spatial gradients of strain in nanocrystalline and associated with the plastic inhomogeneity [28]. To analyze the influence of strain gradient on the mechanical response of nanocrytalline materials, a composite model is developed and employed widely [29]. They divided the nanocrystalline solids into two parts, GI treated as an ordered crystal phase and GBAZ regarded to be plastically softer with respect to strain gradient. Then a strain gradient plasticity theory has been employed to achieve the mechanical properties of nanocrystalline [30], and the theory has been widely applied in characterizing mechanical behaviors of bimodal nanocrystalline materials [31], hierarchically nanotwinned face-centered cubic metals [32], and so on [33].

To highlight the role of CNT in the microstructure of nano/ultrafine-grained matrix, a composite model containing GI and GBAZ will be established with CNT located at GBs and atomically disordered regions near the reinforcement. In this model, the effect of the reinforcement on the thickness of GBAZ is considered and the distribution of GNDs induced by thermal mismatch is assumed to be limited in GBAZ. In addition, the effects of variation of the thickness of CNT-containing GBAZ on the strengthening mechanisms and overall mechanical response have also been introduced. The developed model is validated in comparisons with various experimental results to ensure its applicability in the wide range of CNT-reinforced nano/ultrafine-grained MMCs.

2. Description on the model of CNT-reinforced nano/ultrafine-grained MMCs

2.1. Structure of the two-phase composites

Fig. 1(a) shows the cross-sectional SEM image of 5 vol% CNT-reinforced Cu matrix composites [19]. In this image, the entire composites are obviously divided into two parts, and pure metal matrix is surrounded by the CNT-containing domains. Inspired by the experimental micrograph and the observations that CNT is mostly located at GBs in MMCs [18,20], a two-phase composite morphology has been constructed, schematically shown in Fig. 1(b).

On basis of the concept of nanocrystalline materials, the composites will be converted to the assemblage of spherical particles, as shown in Fig. 2(a), wherein the inner circles, to be denoted as phase 0, represent CNT-free GI, surrounded by CNT-containing GBAZ, to be denoted as phase 1. If the matrix grain size d, thickness δ_{GBAZ} of GBAZ and content f_r of CNT are given, the volume fractions of GI and GBAZ (f_{GI} and f_{GBAZ}, respectively) can be defined as:

$$f_{GI}=\left(\frac{d-\delta_{GBAZ}}{d}\right)^3(1-f_r),\ f_{GBAZ}=1-f_{GI}-f_r \tag{1}$$

Before discussing the overall elastoplastic response of the composites, we will first pay attention on the local microstructure of CNT-containing GBAZ (phase 1), as shown in Fig. 2(a). The reinforcement is assumed to be evenly distributed in this phase. The volume fractions of CNT and GBAZ in phase 1 are denoted as $f_r^{(1)}$ and $f_{GBAZ}^{(1)}$, and the relations between them are established:

$$f_1=f_r+f_{GBAZ},\ f_r^{(1)}=\frac{f_r}{f_1},f_{GBAZ}^{(1)}=\frac{f_{GBAZ}}{f_1} \tag{2}$$

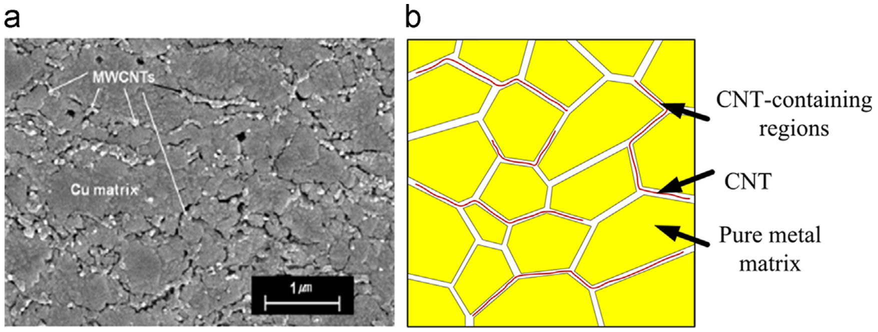

Fig. 1. (a) A cross-sectional SEM image of 5 vol% CNT-reinforced Cu matrix composites [19]; (b) the two-dimensional composite structure of CNT-reinforced MMCs with CNT-free regions surrounded by CNT-containing domains.