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Failure mechanisms in pre-cracked Ni-graphene nanocomposites

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ABSTRACT

Graphene is a 2-D material with superior mechanical properties and is highly desirable as a filler in nanocomposite materials. However, the mechanical properties of the resulting nanocomposite are anisotropic, with strengthening or weakening depending on the loading direction. The presence of graphene also introduces new failure mechanisms to the matrix it is embedded within. In addition, the structure of graphene, pristine or polycrystalline, can affect its interfacial properties in the nanocomposite. We use molecular dynamics to predict the failure mechanisms of Ni-graphene nanocomposites for different loading directions with a crack present in the Ni matrix. We observe a variety of failure mechanisms including dislocation nucleation, graphene bond breaking, and delamination. We also compare the yield stress and strain of nanocomposites with either pristine or polycrystalline graphene. We find that graphene of either kind can improve the yield stress of Ni by 27–76% when loaded parallel to the graphene sheet. We also find that, compared to pristine graphene, polycrystalline graphene can improve the yield stress of a Ni-graphene nanocomposite by up to 27%. This is explained by the higher interfacial shear stress of polycrystalline graphene on Ni's (1 1 1) surface compared to pristine graphene. This is in part related to the wrinkling of graphene sheets, which differs between polycrystalline and pristine sheets. Our research indicates that metal-graphene nanocomposites benefit from graphene's polycrystalline structure when superior mechanical properties are desired.

1. Introduction

For many of its potential applications graphene of a near-pristine structure is desirable. However, producing pristine monolayered graphene sheets is an ongoing challenge for manufacturers of graphene. Generally, graphene sheets have a polycrystalline structure. Studies have shown that the grain boundaries present in polycrystalline graphene lead to lower strength compared to pristine graphene [1–5]. However, depending on the grain structure, graphene's strength may be only slightly diminished [6–8], or can even show some improvement [9].

As a 2-D material, graphene has an incredibly high aspect ratio and specific surface area, which makes it an attractive candidate for use in nanocomposite materials [10]. Research has shown that the inclusion of graphene provides metal matrixes with greatly enhanced mechanical properties [11–16]. Part of the enhancement that metal-graphene nanocomposites show is greater resistance to some failure mechanisms. Kim et al. showed both experimentally and computationally that dislocations are inhibited by graphene sheets, preventing plastic deformation from propagating between regions within a metal matrix separated by graphene [12]. This has been shown to occur under both

indentation [17], tension [18], and compression [19].

Not all failure mechanisms of metal-graphene nanocomposites show improvements over pure metal. The presence of graphene makes delamination a prominent failure mode at the metal-graphene interface [20–22]. The propensity for delamination depends in part on stress concentrations present in the matrix due to defects, like cracks, which ultimately produce dislocations. Dislocations in the metal matrix pile up at the graphene sheet, where stress further concentrates until delamination is initiated [18].

Experiments have shown that graphene's ability to improve the mechanical properties of a nanocomposite is dependent on its ability to transfer load between different regions of the matrix in which it is present [23–25]. Computational work by Sharma et al. has shown that graphene is more effective at load transfer within a matrix than carbon nanotubes, particularly at higher temperatures [26]. The efficiency of graphene's load transfer is dependent on the interfacial shear stress between graphene and the surrounding matrix [27–29]. Wrinkles present in graphene may affect interfacial shear stress by changing the degree of contact between graphene and the matrix. Previous research shows that graphene sheets tend to wrinkle [30–32], and that this can dramatically affect their mechanical properties [33–36]. Yang et al.

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studied fracture in nickel-graphene nanocomposites using MD simulations and found that slip at the nickel/graphene interface and wrinkling in the graphene sheet changed the stress distribution along the graphene layers [16]. This led to a release of stress in metal layers near the graphene sheet. We note that their study considered only pristine graphene, hence different mechanisms that would arise due to polycrystalline graphene remain unexplored.

The presence of graphene will affect the yield behavior of metal matrixes possessing preexisting cracks, but the way that loading and crack orientation affects failure mechanisms of such nanocomposites has not yet been considered. In addition, the effect that the structure of graphene (pristine or polycrystalline) has on the strength of nanocomposites needs further study. This research uses molecular dynamics to predict the yield stress and strain for nanocomposite samples consisting of a pre-cracked Ni matrix with either pristine or polycrystalline graphene sandwiched within it. We consider the failure mechanisms of the nanocomposites under tension with different loading directions and crack orientations. Our previous study [18] used a single crack orientation and loading direction and only pristine graphene.

The novelty of this research is in comparing the mechanical properties of polycrystalline graphene to pristine graphene in the context of metal matrix nanocomposite. This includes comparing the interfacial shear stress between Ni and either pristine or polycrystalline graphene and how the stress field from the crack tip interacts with the graphene. Moreover, we compare the wrinkling of pristine and polycrystalline graphene sandwiched in a Ni matrix; we also analyze the effect this has on the stress distribution of contiguous Ni layers. The results of this study will be important in the context of nanocomposites because polycrystalline graphene is what is generally used in experimental graphene-based nanocomposites. Computational studies of nanocomposites that model only pristine graphene may neglect important effects inherent in graphene's polycrystalline structure and its unique characteristics within matrixes.

2. Methods

In this study, we use molecular dynamics (MD) method to predict the yield stress of a Ni-graphene nanocomposite with an embedded elliptical crack depending on its loading direction, crack orientation, and graphene structure. Yield occurs by either dislocation nucleation within the Ni matrix or delamination of the graphene sheet from the Ni matrix. We compare these results to Ni samples with no graphene included.

2.1. Ni matrix and description of different cases

We choose Ni as the metal matrix in the nanocomposite because the lattice constant for graphene is similar to that of Ni's (1 1 1) face, giving graphene a strong adhesion to the Ni surface [37–39]. For each simulation cell the x , y and z axes correspond to the lattice vectors [1 1 $\bar{2}$], [1 1 1], and [1 $\bar{1}$ 0] respectively. We employ periodic boundary conditions at each boundary. A typical simulation cell for this study is shown in Fig. 1(a). The Ni matrix has an elliptical crack introduced by selective atom removal, with the crack oriented such that its major axis is parallel or perpendicular to the graphene sheet, as shown in Table 1. In all simulations, we deposit graphene on the Ni's (1 1 1) plane, which is the x - z plane. Each simulation cell has either zero, one or two sheets present, as shown in Fig. 1(b). The dimensions of the simulation cell are approximately $500 \times 500 \times 20$ Å. The cracks present in the metal matrix are through-thickness elliptical cracks, with a crack length of 100 Å and an initial opening of 25 Å.

Loading during the simulation can occur either in the x direction, parallel to the graphene sheet, or in the y direction, normal to the graphene sheet. In both cases the elliptical crack in the Ni matrix can be oriented such that its semi-major axis is either parallel with or normal to the graphene sheet. This gives four distinct cases of loading direction

and crack orientation that are organized and shown in Table 1. For case 1 the loading direction and crack orientation are in the x direction, parallel to the graphene sheet. For case 2 the loading direction is the x direction, parallel to the graphene sheet, while the crack is oriented in the y direction, normal to the graphene sheet. For case 3 the loading direction is in the y direction, normal to the graphene sheet, while the crack is oriented in the x direction, parallel to the graphene sheet. For case 4 both the loading direction and crack orientation are in the y direction, normal to the graphene sheet. Each of these cases is considered in this simulation because the relationship between crack and loading direction relative to the graphene sheet plays a major role in the potential failure behavior of the Ni-graphene nanocomposite. When the loading direction and crack orientation are parallel to one another there is no strongly defined crack tip, which occurs for cases 1 and 4. When the loading direction and crack orientation are orthogonal to one another the crack forms a defined crack tip at which stress concentrates, which occurs for cases 2 and 3.

2.2. Graphene layout in pristine and polycrystalline model for single grain boundary

Samples with graphene present are generated with either one or two sheets. A single pristine or polycrystalline graphene sheet is sandwiched within a Ni matrix by first removing a single close-packed layer of Ni atoms around 75 Å below the center of the elliptical crack. For samples with two sheets present, a second sheet is inserted 75 Å above the center of the elliptical crack. This distance allows stress concentration build-up at the crack tip to affect the graphene sheet, but won't lead to dislocations before general failure begins [18]. A pristine sheet is a graphene sheet where all the graphene has one orientation that is continuous at the periodic boundary. A polycrystalline sheet has a regularly oriented graphene region (graphene which is oriented in the same direction as pristine graphene), and a misoriented region. These two regions meet at one grain boundary centered beneath the elliptical crack in the Ni matrix, and one grain boundary located at the periodic interface.

Polycrystalline graphene sheets are created for the model by first generating an oversized graphene sheet for each desired grain. Grains are then cut from the oversized sheet in the shape desired for the final grain structure. Regularly oriented grains have a symmetric periodic image, allowing it to act as a single unbroken grain. Misoriented grains have a nonsymmetric periodic image, which means that an additional grain boundary is formed at the simulation cell's periodic boundary. Thus, each regular grain only has two boundaries, each parallel to the z axis, while each misoriented grain has four different boundaries, two parallel to the z axis and two parallel to the x axis. Since no loading is done parallel to the z axis, the stress concentration generated at the misoriented grain's periodic boundary is minimal compared to the stress concentration at the regular-grain/misoriented-grain interface. A regularly oriented grain is a grain with an orientation of 0°. Angles for the misoriented grains are chosen based on experimental observation of polycrystalline graphene sheet orientations [40] which found that grains with misorientation angles closer to 0° and 30° were more common than middle range angles, though middle range angles were still present. Additionally, polycrystalline graphene sheets with high angle grain misorientations have been shown experimentally to have higher strength than graphene sheets with lower angle grain misorientations [7]. We use misoriented angles of 15° and 30° to encompass both less common and more common misoriented boundaries, as well as sheets that have lower and higher strength. An example of the regular-grain/misoriented-grain boundary is shown in Fig. 2. Note that the defects we see at our polycrystalline grain boundary are similar to the Stone-Wales defects that have been observed at polycrystalline graphene grain boundaries both computationally [41] and experimentally [40].

The rectangular straight-edged grain boundaries in our

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