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RELAXATION OF THERMAL MISMATCH IN DISCONTINUOUSLY REINFORCED COMPOSITES

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Abstract

We have measured the dislocation density and thermal residual elastic strain in NiAl matrices of 20 vol. pct. (V%) Al_2O_3 discontinuously-reinforced composites. As the size of the reinforcement increases the average dislocation density increases, and the corresponding thermal residual elastic strains decrease. The changes with respect to particle size in the dislocation density and residual strain can neither be explained by continuum theory nor by dislocation mechanics for a homogeneous medium. A previously developed model (that satisfactorily describes the SiC/Al system) suggests that the misfit dislocation density decreases with increase in reinforcement size but this disagrees with the current Al_2O_3/NiAl results. A new model is proposed to describe low-symmetry intermetallics, which are constrained in their ability to relax thermal mismatch because of a paucity of independent slip systems. The results are discussed in the context of continuum mechanics using finite element analyses and crystal plasticity.

Introduction

In ceramic reinforced metal matrix composites (MMCs), dislocations are generated during cooling from fabrication temperatures because the coefficients of thermal expansion of the constituents are incompatible [1]. The generation of dislocations has been investigated in several composites such as SiC/Al, Al_2O_3/NiAl and TiB_2/NiAl [1-3].

Several models have been developed to predict the resultant dislocation density, or a continuum equivalent—the average effective plastic strain [4,5]. For example the prismatic punching model developed by Arsenault and Shi [4] predicts that: (1) dislocation density increases with reinforcement volume fraction; and (2) for a constant reinforcement volume fraction, the dislocation density decreases with increasing particle size. These predictions follow because the mismatch prismatic dislocation density is proportional to the total particle surface area. Experimentally the changes in mismatch dislocation density in SiC/Al MMCs follow the prismatic punching model as shown in Fig. 1, $\rho \propto D^{-\alpha}$ [4,6] where D is the particle size.

In polycrystalline low-symmetry intermetallics such as NiAl, slip in individual grains is impeded by a paucity of independent slip systems and the constraint of the neighboring grains. Therefore, the generation of thermal mismatch dislocations is limited by these slip constraints. As in aluminum-based MMCs (where a high dislocation density is beneficial to strengthening), a high density of mobile dislocations in intermetallic composites is desirable for enhancing the ductility. In this investigation, matrix thermal residual elastic strains and matrix dislocation densities were determined in Al_2O_3-reinforced NiAl using neutron diffraction and transmission electron microscopy (TEM), respectively. The effects of different reinforcement sizes and morphologies were examined and compared with SiC/Al MMCs.

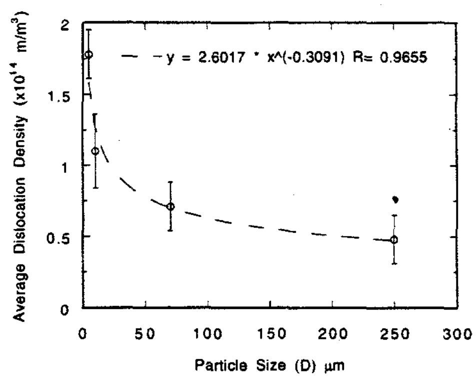

Figure 1 Average matrix dislocation density in annealed 20 V% SiC/Al composite as a function of particle size.

Experimental Procedure

Five 20V% Al_2O_3/NiAl samples were produced with varying reinforcement sizes and shapes; equiaxed particles (hereafter referred to as spheres) with diameters of 5, 75, 355 µm, short fibers and continuous filaments. For the 5 and 75 µm spheres matrix and reinforcement powders of the same size were blended during premixing. For the 355-µm spherical and short-fiber (diameter of 10 µm and average aspect ratio of 10) composites, 75 µm NiAl powder was premixed. The powder mixtures with different particle sizes and morphologies were separately hot pressed at 1623 K for 4 hours at 25 MPa. The continuous filament (diameter of 144 µm) composite was fabricated by a powder cloth technique. All samples were annealed at 1673 K for between 1 and 4 hours followed by furnace cooling. Since a similar powder metallurgical procedure was applied to the fabrication of all specimens (except the filament composite), the as-processed matrix microstructure should be similar in all cases (detailed grain size is not yet available due to a lack of suitable etching solution).

TEM analyses were performed with operating voltages of 200 KV and 1 MV. Sample preparation and data analysis are described elsewhere [7]. Thermal residual elastic strains were measured using the high resolution powder diffractometer at the ISIS facility of the Rutherford Appleton Laboratory, UK. Elastic strains were determined from changes in the lattice constants of the composite matrix (NiAl) with respect to a strain-free reference. Lattice constants (a) were determined by fitting of the complete diffraction patterns that are determined in a time-of-flight measurement using Rietveld refinement [8]. During the refinement a starting diffraction pattern is constructed from the crystal structures of all phases. The lattice spacing (d_{hkl}) is then least-squares-fitted to the neutron data without alteration of the crystal structures. The results represent the best crystallographic equivalence of an aggregate of homogeneously deforming crystals to the real specimen. More details were described by Bourke et al. [9,10]. FEM modeling was performed using ABAQUS™. Meshes representing two dimensional axisymmetric unit cells containing spherical, short and continuous cylindrical reinforcements were constructed with periodic boundary conditions. A similar procedure is described elsewhere [5,11].

Results

The dislocation densities obtained by TEM for the various shapes and sizes of the Al_2O_3 reinforcement are shown in Figs. 2a and 2b. Although the data are limited, the increase in dislocation density with reinforcement size, as well as between discontinuously reinforced (spheres and short-fibers) and continuous filament is apparent. Comparing Fig. 2b with Fig. 1, the changes in dislocation density as a function of the reinforcement size show opposing trends for the Al_2O_3/NiAl and the SiC/Al. Furthermore, the dislocation density for the 75 μm (spherical particle) composite is higher than that for the short-fiber composite (Fig. 2a), despite the fact that the total matrix/reinforcement interface area for the latter is more than five times larger than that for the former. This contradicts predictions from the prismatic punching model, which predicts an increase in dislocation density with total interface area.

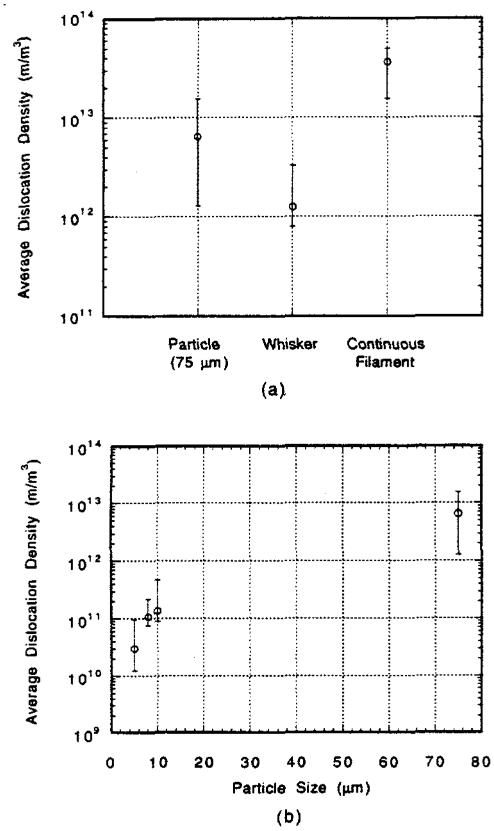

Figure 2 Average matrix dislocation density in annealed 20V% Al_2O_3/NiAl composites as a function of (a) particle shapes, and (b) particle sizes for the spherical composites. The error bar represents the range of data scatter.

Figure 3 shows FEM results relating reinforcement morphology to the average matrix effective plastic strain. Although the effective plastic strain is not expected to vary with the *size* of the reinforcement, it increases as the reinforcement *morphology* progresses from spherical to short-fiber to continuous-filament. Assuming that a fixed portion of the distortion energy is associated with the generation of dislocations (i.e. the dislocation density is proportional to the volume averaged effective plastic strain), the trend of the FEM predictions for the short- and continuous-fiber data (Fig. 3) is consistent with the TEM results (Fig. 2a). However, the continuum (FEM) results in Fig. 3 indicate that the short-fiber composites should be associated with more plasticity than the spherical composite during cooling. As with the prismatic dislocation model, the dislocation densities on the changes from spherical to short-fiber composites (Fig. 2a) disagree with the FEM results.

Table 1 lists the mean phase matrix radial residual elastic strains measured by neutron diffraction in the Al_2O_3/NiAl composites described. During the collection of the neutron diffraction patterns the scattering vectors for all specimens lay in a plane perpendicular to the hot-pressing direction. With planar-isotropism perpendicular to the pressing direction, diffraction results are expected to be independent of any directional anisotropy associated with the pressing procedure. The mean phase residual strains decrease as the particle size increases, but there is a significant increase as the reinforcement morphology changes from equiaxed particles to short fibers. Unfortunately suitable standards were not available for measurement of residual strains in the Al_2O_3. Previous neutron measurements of these composites also show that the radial thermal residual stress for the continuous filament composite is smaller than that of the short-fiber composite (238 MPa for the continuous filament composite [12] and 383 MPa for the short-fiber composite [13]).

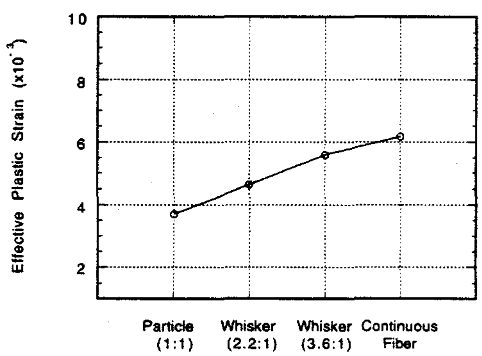

Figure 3 Effective plastic strains predicted by FEM for different reinforcement shapes (particle size does not influence the results).

Table I Matrix Radial Thermal Residual Strain In Al_2O_3/NiAl Composites

Reinforcement (Al_2O_3)Size	Matrix Radial Residual Strains (10^{-4})
5 μm	4.6±0.077
75 μm	3.7±0.098
355 μm	0.87±0.098
Short fiber	8.2±0.098

Comparing the residual strains with the FEM prediction the following trends can be observed: (1) residual strains being dependent on the particle size disagrees with the FEM results; (2) the changes of residual strain from spherical to short-fiber composites agree with FEM results [2]; and (3) the changes of residual stresses from short- to continuous-fiber composite are inconsistent with the FEM. Although no clear trend can be identified as how the experimental results compares with the models, the dislocation and residual strain data suggest that a single parameter, reinforcement size, dictates the plastic relaxation of thermal mismatch in NiAl composites. The larger the reinforcement size, the more complete the plastic relaxation.

Discussions

Plastic relaxation through dislocation generation requires that thermal mismatch generates stresses that are higher than the matrix critical resolved shear stress (CRSS). Figure 4 shows an FEM prediction of the unrelaxed octahedral shear stress generated by the thermal mismatch, and the uniaxial yield stress for polycrystalline NiAl. The Von Mises yielding criterion is exceeded at all temperatures. This suggests that plastic flow must occur in the NiAl matrix if the principles of phenomenological continuum theories are applicable. The particle-size dependency of the residual strain in the NiAl / Al_2O_3 suggests that although the plastic relaxation does take place, it is very dependent on the microstructural parameters, which cannot be accounted for by continuum theories.

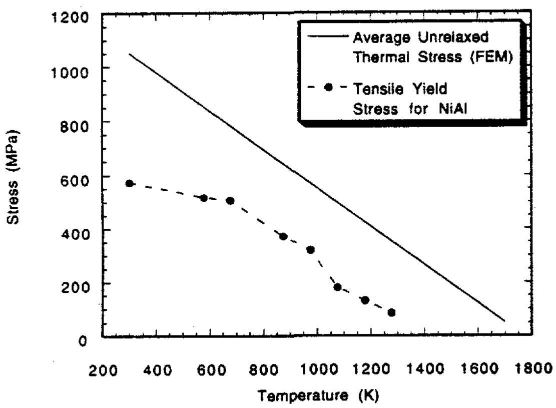

Figure 4 Experimentally measured yield stress of unreinforced polycrystalline NiAl at different temperatures and the predicted matrix thermal mismatch octahedral shear stress without plastic relaxation (elastic matrix).

To understand the difference in SiC/Al and Al_2O_3/NiAl composites with respect to their mismatch dislocation density vs. particle size relationships (Figs. 1 and 2b), one must consider the slip characteristics of the two matrices. Aluminum has an fcc crystal structure with 12 different slip systems of which five are independent. This allows each individual grain to slip independently. In NiAl where the predominant slip system is <100>{100} there are only three independent slip systems [14] with the hard orientation along <100> and the soft orientation along <110> and <111>. The difference in the CRSS between "hard" and the "soft" orientations is about a factor of 14 [15]. According to Von Mises [16], however, self-contained slip within an individual grain of a polycrystalline material requires five independent slip systems without sacrificing intergranular deformation compatibility. Therefore, to avoid creating discontinuities in the NiAl matrix, plastic deformation can occur only when collaborative slip between neighboring grains is activated. This is facilitated when the misfit thermal stress field associated with the reinforcement particles encompasses a greater number of matrix grains, in which case, slip in a particular grain is more likely to be accommodated by flow in other grains.

Figure 5 shows two cases in which the reinforcement size is larger (Fig. 5a) and smaller (Fig. 5b) than the surrounding matrix grains. Due to thermal misfit, a mismatch-affected zone (MAZ) exists around each particle within which a misfit stress develops. The size of the MAZ is proportional, to first order, to the particle size. Thus when the particle size increases relative to the matrix grain size, more matrix grains are encompassed by the MAZ. Then the CRSS is exceeded in many matrix grains and the probability of some having favorable crystallographic orientations for collaborative multi-grain slip increases. Conversely when the reinforcement particle size decreases relative to the matrix grain size, the number of grains in the MAZ reduces and the probability of a favorable grain arrangement for collaborative slip decreases. Thus for a relatively constant matrix grain size plastic relaxation is more likely for large reinforcement particles, supporting the experimental results in this work. Numerical models employing crystal plasticity of polycrystalline aggregates are needed to provide further quantitative understanding of this process.

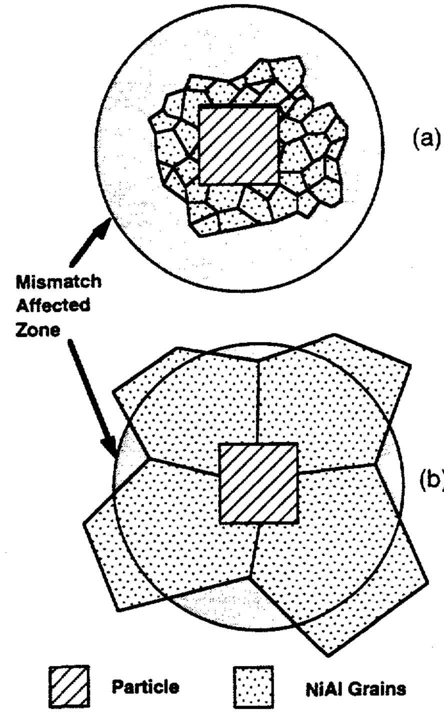

Figure 5 Mismatch affected zone (MAZ) within which large thermal misfit develops. (a) The MAZ is much larger than matrix grains (large particles with constant grain size); (b) the MAZ is much smaller than matrix grains (small particles with constant grain size).

The results reported in Table 1 are derived from changes in the bulk lattice parameters which provide a mean phase average of the residual strain. However this approach of using the Rietveld method hides the anisotropy associated with individual reflections. Single peak fits show that strains along individual directions can vary considerably. For example, in all samples the strains derived from the [100] and [110] reflections are consistently larger and smaller, respectively, than the average from the overall refinement. This indicates more retained thermal mismatch along the hard orientation (less plastic relaxation), and less along the soft orientation (more plastic relaxation). That is, plastic relaxation is grain and orientation sensitive, and is consistent with the deformation mode suggested above. More quantitative analysis of the diffraction data will be reported elsewhere.

The decrease of thermal residual strain with increasing particle size in the Al_2O_3/NiAl composites is also consistent with the deformation modes of multigrain-slip in NiAl. Although continuum theory predicts an invariance of field quantities to particle size nevertheless the *apparent* polycrystalline yield stress increases with a decreasing particle size when the collaborative slip requirement is impeded in the crystal aggregates. More unrelaxed thermal mismatch is retained in the NiAl with a higher *apparent* polycrystalline yield stress, i.e. a higher thermal residual strain. The residual strain results are also consistent with the TEM dislocation measurements. Therefore, the intergranular-collaborative-slip argument presented herein supports the suggestion that, with relatively constant matrix grain size, the reinforcement size is the single most important parameter that determines the extent of plastic relaxation of thermal mismatch in low-symmetry intermetallic composites.

Conclusions

- In Al_2O_3/NiAl composites the matrix dislocation density from relaxation of thermal mismatch *increases* as the Al_2O_3 particle size increases. In contrast, matrix dislocation density in SiC/Al composite *decreases* as SiC particle size increases.
- The contrast in the dislocation density/particle size relationship for the two composites suggests that plastic relaxation in low symmetry polycrystalline NiAl requires collaborative slip between grains.
- Neutron diffraction results indicate that matrix thermal residual strains in Al_2O_3/NiAl composites decrease as particle size increases, consistent with the variations of dislocation density obtained from TEM.
- The concept of multigrain collaborative slip suggests that the particle size relative to the matrix grain size is the single most important parameter in determine the extent of plastic relaxation of thermal mismatch in low-symmetry intermetallic composites.

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