Interface constitutive and its impact on mechanical properties of magnesium-matrix ceramic particle reinforced nanocomposites

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Abstract

The interface mechanical behavior of the magnesium matrix composite reinforced by silicon carbide nanoparticles (Mg/SiC nanocomposites) and the influence of interface constitutive characteristics on its macroscopic tensile properties have been studied systematically by using a multi-step simulation approach based on ab initio/molecular dynamics/finite element. The interfacial potentials for Mg/SiC interfaces are derived from ab initio adhesive energies by an inversion method firstly. The generated interfacial potentials are then applied to molecular dynamics (MD) simulations to parameterize the cohesive zone model (CZM) and obtain the traction-separation law for the Mg/SiC interface under mixed mode loadings. The finite element simulations based on the parameterized CZM are finally conducted to predict the macroscopic stress-strain response of the Mg/SiC nanocomposites under quasi-static tensile loadings and compared with experimental results. Our macromechanical property predictions agree very well with earlier research work [1]. Additionally, the multi-step checks show that these inversion potentials are self-consistent, further confirming the validity of the simulated interface constitutive behavior and macromechanical response with interface effect. These inversion potentials may have significance for some complex metal-ceramic interface structures.

Keywords: Metal-matrix nanocomposites, Interfacial potentials, Mechanical properties, Multi-step simulation.

Determination of Pair Potentials and CZM Model

Figure 1(a) shows the resultant potential curves of Φ_{Mg-Si} and Φ_{Mg-C}, which are derived from the adhesive energies by using the final inversion formula; while Figure 1(b) shows the comparison between the original *ab initio* adhesive energy and the ones calculated by the inversed potentials. These two potentials can be furtherly fitted into the Morse potential.

Figure 2 shows three dimensional shear and normal stresses as functions of crack opening displacement and mixed-mode loading angle by using the derived interfacial potentials in MD simulations.

Validation of the CZM by FEA

A comparison between simulated and experimental stress-strain curves of the composites with different weight percentages is represented in Figure 3. This figure clearly proves that the simulated results are in excellent quantitative agreement with the experiments.

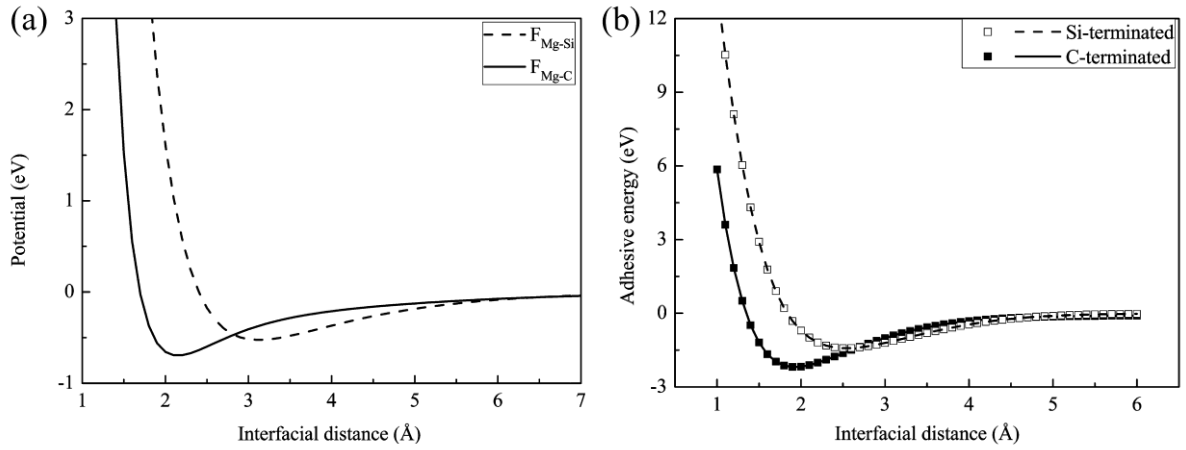

Figure 1. (a) The inversion potential curves of $\Phi_{Mg\text{-}Si}$ and $\Phi_{Mg\text{-}C}$; (b) comparison between the adhesive energies calculated by either *ab initio* method or the inversion potentials. The squares indicate the *ab initio* results and the lines denote the sum of inversion pair potentials

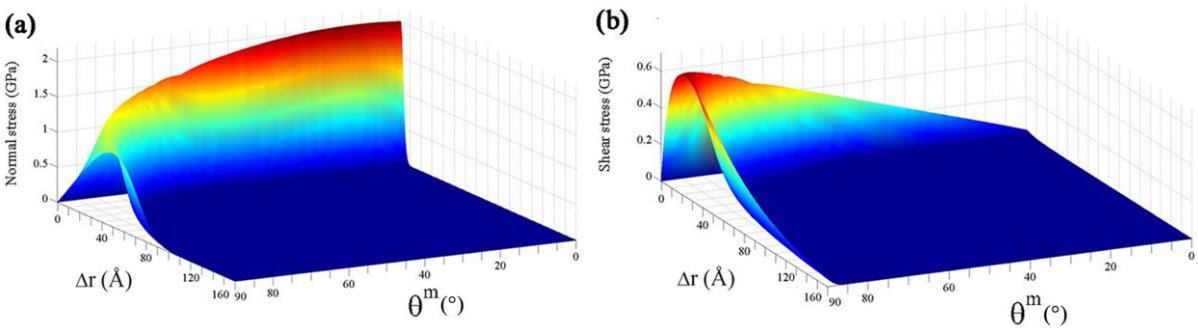

Figure 2. Surface plot of stress as a function of local loading angle θ^m and crack opening displacement Δr. (a) Normal stress and (b) shear stress

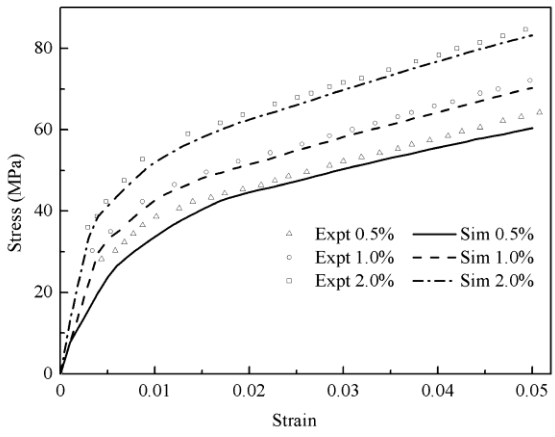

Figure 3. Comparisons between simulated and experimental results [1]

Acknowledgments

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References

[1] Cao, G., Konishi, H. and Li, X. (2008) Mechanical properties and microstructure of Mg/SiC nanocomposites fabricated by ultrasonic cavitation based nanomanufacturing, *Journal of Manufacturing Science and Engineering* **130**, 031105–1–031105–6.