

## DIFFUSION EFFECT ON THE COHESIVE ZONE MODEL OF SiC/Al INTERFACE USING ATOMISTIC SIMULATIONS

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### ABSTRACT

Metal matrix composites (MMCs) are materials consisting of a metal matrix reinforced often with ceramic to improve the properties of the base metal. MMCs are used in a wide range of applications due to their unique combination of high strength, stiffness, and wear resistance with relatively low weight.

It is well recognized that the interface in composites plays a crucial role in transferring the load efficiently from the matrix to the reinforcement. Hence, to predict the overall mechanical properties of MMCs, it is essential to evaluate the interface strength. In this study, the C- and Si-terminated hexagonal and cubic SiC/Al interfaces are studied. The molecular dynamics (MD) simulation is used as a virtual environment to obtain this relation because it is challenging to determine it from experimental results. The equivalent mechanical properties of the interface are characterized by a cohesive zone model based on the traction-separation relation obtained from MD simulations. SiC/Al composites are created using high-temperature techniques that result in a fuzzy interface due to the diffusion of atoms [1]. In this research, the effect of diffusion on the traction-separation relation in mode I fracture is examined. The systems are heated to 2000 K and then cooled to 300 K. Young's modulus of samples after atom diffusion is found to be about 25% lower than those before atom diffusion, but the work of separation is found to increase by at least 40% following the heating of the system and diffusion. This finding demonstrates that diffusion significantly increases the fracture energy of SiC/Al composites. Furthermore, following system heating and diffusion of atoms, the C-terminated samples are found to have higher work of separation than the Si-terminated ones.

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### REFERENCE

- [1] Tahani M., Postek E., Sadowski T., *Molecular dynamics study of interdiffusion for cubic and hexagonal SiC/Al interfaces*, Crystals, Vol. 13 (1), 46, 2023.