Society of Engineering Science 51st Annual Technical Meeting

1–3 October 2014

Purdue University, West Lafayette, Indiana, USA

An ab-initio analysis of the influence of knock-on-atom induced damage on the peak tensile strength of 3C-SiC grain boundaries

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ABSTRACT

The effect of knock-on atom induced damage on the peak tensile strength of cubic silicon carbide (3C-SiC) is examined using an ab initio simulation framework based on Car Parrinello Molecular Dynamics method. The framework examines the effect of impact damage caused by a knock-on atom with velocities corresponding to four different kinetic energy levels (50 eV, 500 eV, 1 keV, and 2 keV) in three different SiC structure samples with different grain boundary (GB) configurations. Analyses show that peak tensile strength of the examined structures decreases by up to 37% in samples with GBs due to the impact damage caused by knock-on atom when compared with the case of single crystalline SiC under similar conditions. Analyses reveal new insights regarding the influence of bond strength change under knock-on atom induced impact damage on peak tensile strength of the examined structures. It is found that the peak tensile strength of the examined structures is a function of change in temperature, impact energy, and GB configuration. In order to extend the observed correlation of the peak tensile strength with atomic configurations to other structure types, a fractal dimension-based approach is adopted to predict structure peak tensile strength as a function of knock-on atom impact energy, temperature, and GB configuration. Analyses show that the tensile strength of the examined SiC structures increases as a function of their fractal dimension increase. Fractal dimensions also change as a function of change in impact energy level and the corresponding damage in an inversely proportional manner. Based on the observed correlations, an empirical relation to predict structure peak tensile strength as a function of simulation parameters is developed. The developed relation is found to predict strength data of structures not included in the fitting with good accuracy.