Molecular simulations of ultrafast radiation induced melting at metal-semiconductor interfaces

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Understanding radiation induced ultrafast melting at material interfaces is essential in designing robust electronic devices for aviation/space applications and in laser machining. While it is difficult to achieve the spatial and temporal resolution required to quantify the phenomenon experimentally, simulations can provide the detailed mechanisms of the structural changes that happen during phase transition. In this work, we use molecular simulations to study the effect of radiation damage on silicon carbide (SiC) - tungsten (W) interfaces which is of interest in high power electronics. A multi-scale approach is involved wherein the reactions at the interfaces are quantified using *ab-initio* molecular dynamics (MD) simulations and classical MD simulations are employed to understand the structural and diffusional changes across the material interface. Finally, coarse-grained Lennard-Jones type models are used to study the larger scale mechanisms and structures obtained due to the induced damages. We show that the response of the material to radiation damage depends on factors such as energy of the incident radiation, thermal properties, and molecular structure of the material.