

Investigation of excitation-induced non-thermal effects in semiconductors, metals and alloys

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Excitation-induced non-thermal melting in silicon, as well as bond-hardening in gold following strong laser irradiation with short pulse durations have been known for several years [1]. Furthermore, several traces of excitation-induced solid-solid phase transitions have been noticed in a variety of materials.

Here, we present several approaches to identify and quantify excitation-induced effects changing the bond strength and inducing phase transitions systematically in several semiconductors, metals and alloys obtained from DFT calculations depending on the degree of excitation. These calculation are in line with previous investigations and provide new insights into the change of the bond strength and the induced phase transitions following strong laser excitation.

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References: [1] V. Recoules, J. Clérouin, G. Zérah, P.M. Anglade, S. Mazevet. Effect of intense laser irradiation on the lattice stability of semiconductors and metals. Phys Rev Lett. 2006 Feb 10;96(5):055503. doi: 10.1103/PhysRevLett.96.055503.