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Two-Temperature Modeling of Swift Heavy Ion Effects from First Principles

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The inelastic thermal spike model[1] has been widely used to describe the effects of swift heavy ions, but its theoretical suitability remains under debate[2]. The parameters for the underlying mathematical equations, the so called two-temperature model (TTM) equations, are typically obtained from empirical fits to ion track radii. Recent computational advances now make it possible to determine these parameters from first principles using density functional theory combined with semiclassical transport theory. The TTM can be viewed as an approximation to the semiclassical electron–phonon transport equations, namely the Bloch–Boltzmann–Peierls equations. We calculate TTM parameters from first principles to construct a model directly grounded in semiclassical transport theory, and apply it to materials such as diamond, quartz, and various metals. This approach will help assess whether electron–phonon coupling alone explains ion track formation or if additional mechanisms must be invoked.

Literature:

[1] M. Toulemonde et al. Nucl. Instrum. Methods Phys. Res. B 2012, 277, 28-39
[2] Medvedev et al. J. Appl. Phys. 2023, 133, 100701

Author: LEINO, Aleksi (University of Helsinki)

Co-authors: ZVEREV, Alexei (University of Helsinki); GRAHAM, Joseph (Missouri S&T); DJURABEKOVA, Fluyra (University of Helsinki)

Presenter: LEINO, Aleksi (University of Helsinki)

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