Seminar

Institute for Plasma Research

Title : Assessment of thermal spike model via swift heavy ion mixing

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Abstract :

The thermal spike model (TSM) is presently a widely accepted mechanism of swift heavy ion (SHI)- matter interaction. Although there have been attempts to verify the validity of the model via a number of ion fluence dependent studies of SHI induced effects and their comparison with TSM calculations, all provide a highly indirect and crude indication of the occurrence of SHI induced processes as hypothesized in the model, and use the free electron theory of metals. This present work relies on an improvement based on the use of density functional theory (DFT), instead, for deriving the key TSM input parameters. The strategy is to (a) use DFT and TSM calculations to demonstrate the variability of the key thermophysical parameters relevant to the SHI-matter interaction, and (b) exploit this variability to assess the TSM via experimental observation of SHI induced mixing. The study has been performed in the following three sequential steps. **Step 1**: This initial step is to perform DFT computations of temperature dependence of e-p coupling strength (G) and specific heat (C_e) in (i) three orientations - [001], [110] and [111] - of thin (~ 16 ˚A) Bi_2Te_3 slabs, and (ii) $Ti_{1-x}Zr_x$ alloy system with different compositions (x = 0, 0.25, 0.5, 0.75, 1). This alloy system is completely solid soluble in low temperature hcp phase and high temperature bcc phase separately. A smooth variation in x dependence of electron density of states can therefore be expected for this system, and thus seeing the variations of the TSM parameters with x would be interesting. This step of the present work demonstrates that the intricate details of electron density of states, as obtainable from DFT computations, do influence the temperature dependence of G and C_e. **Step 2:** This step is meant to select a binary alloy system simpler than $Ti_{1-x}Zr_x$ with which SHI mixing experiments could be feasible. $Pd_{1-x}Ni_x$ is such a prospective isomorphous system for which a systematic x variation of temperature dependences of the two thermophysical parameters is expected. The intention is to investigate whether the interdiffusion of Pd and Si, and that of Ni and Si, on SHI irradiation of $Pd_{1-x}Ni_x$/Si interfaces is feasible. Since SHI induced molten states are necessary for such interdiffusion, the objective of this step narrows down to use the TSM calculations and find if molten state can be induced by SHI's in Pd and Ni, at least in the vicinity of the Pd/Si or Ni/Si interface. 100 MeV Au ions have been chosen for the study. It is found from the TSM calculations that both bulk Pd and bulk Ni are insensitive to 100 MeV Au irradiation. Favourably, however, both Pd and Ni are meltable in the vicinity of the interface in the presence of their interface with Si. **Step 3:** This step is intended to finally assess the TSM. The strategy is to (i) investigate the x variation of C_e and G computed using DFT, and thereby getting an indication of whether an x-variation of mixing could be observable in experiments, (ii) experimentally determine the x variation of efficiency of SHI drivenmixing of Pd and Ni in Si via 100 MeV Au irradiation of $Pd_{1-x}Ni_x$/Si system, (iii) qualitative estimate the x dependence of extent of mixing using the computed C_e and G values and the TTM equations, and (iv) make a comparison between the experimental and computational results. Experimentally, the extent of mixing has been parametrized by the irradiation induced change $\Delta\sigma^2$ in variances of Pd and Ni depth profiles derived from x-ray photoelectron spectroscopy. Computationally, G and Ce determined using DFT have been used to solve the equations appropriate to TSM, and then an equivalent quantity L^2, proportional to $\Delta\sigma^2$, has been calculated. Both $\Delta\sigma^2$ (x) and L^2 (x) show non-linearities, albeit in slightly dissimilar ways, leading to a conjecture that the present work at least does not invalidate the TSM.

Keywords: Swift heavy ion-matter interaction, thermal spike model, density functional theory