Abstract Submitted
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Enhancing mechanical toughness of aluminum surfaces by nanoboron implantation: An *ab initio* study[1] ZHEN ZHU, Michigan State University, DAE-GYEON KWON, YOUNG-KYUN KWON, Kyung Hee University, DAVID TOMANEK, Michigan State University — We use *ab initio* density functional theory to study the formation dynamics and equilibrium atomic arrangement in aluminum surfaces exposed to energetic boron aggregates. Results of our molecular dynamics simulations indicate that after using up their excess kinetic energy to locally melt the aluminum surface, boron atoms prefer to remain in subsurface sites. We perform extensive structure optimization studies to identify the optimum structural arrangement and changes in the electronic structure associated with the formation of strong Al-B bonds, which are responsible for the stability enhancement of the compound. Nano-indentation simulations based on constrained optimization suggest that presence of boron atoms enhances the mechanical hardness and wear-resistance of aluminum surfaces.

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