Abstract Submitted
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Alloying and Pressure Effects on Material Strength from First Principles[1] LIN H. YANG, HYUNCHAE CYNN, JAE-HYUN KLEPEIS, JOHN PASK, ROBERT RUDD, Lawrence Livermore National Laboratory, MICHAEL SHAUGHNESSY, University of California,Davis and Lawrence Livermore National Laboratory — It is well known that impurities and alloying can have a profound influence on the strength properties of a material. For example, alloying tantalum (Ta) with 10% tungsten (W) increases the yield strength of the material by more than a factor of two [1]. In this work, we have developed a predictive theory of alloying and pressure effects on material strength from first principles. To be specific, we use $Ta_{1-x} - W_x$ alloy as a prototype system where the generalized stacking fault energies and elastic moduli were calculated from first principles. These results were then used to access the pressure and alloying effects on the relative strength of $Ta_{1-x} - W_x$ alloys. Our results appear to be consistent with the general trend that the alloying effects can have profound impacts on the material strength. With the applied pressure up to 2Mbar, the alloying effects on the strength remain to be very profound.

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