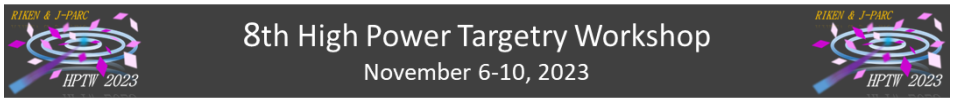

Contribution ID: **47** Type: **Contributed Oral**

Computational Exploration of High Entropy Alloys as Promising Materials for Future Beam Windows

Tuesday, 7 November 2023 09:30 (15 minutes)

Beam power and runtime in high energy particle accelerators face limitations due to targets and beam windows, experiencing thermal shock, fatigue, and irradiation damage from the beam. To achieve higher beam power and extended runtime, the development of new materials is crucial, with High Entropy Alloys (HEAs) emerging as a promising solution due to their exceptional properties, including high strength, ductility, and radiation resistance. This study proposes an integrated approach that combines computational techniques, including CALPHAD, density functional theory (DFT), and molecular dynamics (MD), to comprehensively investigate defect properties of suitable HEAs, offering potential alternatives for the next generation of beam windows. Starting with a previously studied single-phase BCC CrMnV ternary alloy, small quantities of Ti were introduced as an impurity getter, and Al was added to decrease density while, in conjunction with added Co, promoting a coherent B2 phase to strengthen the material with minimal embrittlement. CALPHAD is employed to conduct approximately one hundred thousand simulations, facilitating the identification of potential HEA compositions. Subsequently, a DFT-informed machine learning potential is being developed to analyze the defect properties of the narrowed HEA compositions, and machine-learned potentials will be utilized for running molecular dynamic (MD) simulations to study defect properties in these alloys. This research not only outlines the CALPHAD approach and highlights the importance of DFT in developing HEAs but also demonstrates the promising role of machine learning in this context. The findings from this study hold the potential to significantly advance materials used in high energy particle accelerator components, ultimately leading to increased beam power and improved runtime.

Themes for the contribution

2 Radiation damage in target material and related simulations:

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