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

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With the ever-increasing demand for high beam power, the currently used beam-intercepting devices (BIDs) such as targets, and beam windows may not be able to handle the high power required for future accelerator complexes or the lifetime may be reduced drastically. As beam power increases, the damage incurred by BIDs, including thermal shock, fatigue, and irradiation damage, also rises. Therefore, it is imperative to design materials that can withstand high beam power for longer lifetimes. High entropy alloys (HEAs) have emerged as potential alternative materials for designing next-generation BIDs. In this study, we primarily focus on materials for developing beam windows for next-generation accelerator complexes. We propose an integrated approach that combines various computational techniques to study and design new materials. Specifically, we use CALPHAD, density functional theory (DFT), and molecular dynamics (MD) to comprehensively investigate the defect properties of suitable HEAs, offering potential alternatives for future beam windows. We begin by scanning the extensive phase space provided by Cr-Mn-V-Ti-Al-Co HEAs, selecting 8 compositions after evaluating approximately 120,000 unique compositions using CALPHAD. We, then employ DFT-informed machine learning techniques to develop force-field parameters. Finally, MD simulations using these developed force-field parameters will be used to study the effects of radiation damage on the defect and mechanical properties of the selected alloys. This research explains the use of the CALPHAD approach and shows how critical modeling (DFT and MD) is in developing novel material such as HEAs. It also highlights the promising role of machine learning in this field. The results from this study will greatly improve the novel materials development to be used in next-generation accelerator components, leading to higher beam power and longer operational times of BIDs.

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