NOMATEN Online Junior Seminar

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Title: Plasticity-oriented interatomic potential for CrFeMnNi high entropy alloys
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Abstract: With the increasing demand for materials capable of enduring extreme environments and facilitating technological progress, there has been a concerted effort to explore advanced solutions. This pursuit has led to the emergence of High Entropy Alloys (HEAs) as a promising category of metallic alloys. Recent studies have uncovered the potential of certain HEAs to outperform traditional alloys in terms of various properties. Notably, some HEAs exhibit exceptional characteristics such as high solid solution and strain hardening, decelerated phase transformation kinetics, and improved resistance to radiation. For instance, face-centered cubic (FCC) structured HEAs demonstrate a unique blend of strength and ductility, particularly evident at cryogenic temperatures. Among these, the Cantor alloy, composed of CoCrFeMnNi in equimolar proportions, stands out for its superior resistance to void swelling under irradiation. However, its unsuitability for nuclear applications due to the generation of the 60Co radioisotope during neutron irradiation has spurred research into Cobalt-free alternatives capable of replicating its exceptional properties.

Nevertheless, the precise mechanisms underlying the high strength of certain HEAs remain a subject of debate within the scientific community, with some attributing this phenomenon to dislocation mechanisms. In this study, we investigate the plasticity characteristics of a single-phased austenitic HEA known as Y3-HEA, with a chemical composition of Cr15Fe46Mn17Ni22 (at%). This alloy was recently developed at MINES Saint Etienne, France. Our investigation aims to comprehend the behavior of this alloy under both irradiation and non-irradiation conditions. To elucidate the potential improvements stemming from the complex chemical composition of the material and to underscore the disparities between an HEA and a conventional alloy, we conduct a comparative analysis with a classical austenitic stainless steel (ASS) model alloy Cr20Fe70Ni10 (at%).

Approaching the problem from an atomic-scale perspective, we focus on phenomena such as dislocation mobility and interaction with irradiation defects, which predominantly originate at the atomic level. Our primary emphasis is on the edge dislocation model. Initially, we develop a novel interatomic potential based on the Embedded Atom Method (EAM), specifically tailored for the CrFeMnNi system. This new potential accounts for the presence of Manganese (Mn), which has posed a challenge in previous models. By applying this interatomic potential to molecular statics and molecular dynamics, we observe significant disparities in mechanical behavior between the two studied alloys. Y3-HEA exhibits higher fluctuations in local stacking fault energy (SFE) compared to ASS, resulting in a higher critical stress required to initiate dislocation motion. Through a quantitative assessment of dislocation mobility, we predict slower dislocation mobility in Y3-HEA compared to ASS, suggesting that the interaction of high SFE fluctuations and dislocation mobility may contribute to increased strength and ductility in Y3-HEA.

Moreover, our recent findings indicate that dislocation mobility can be influenced by composition. Additionally, HEAs are anticipated to possess enhanced resistance to irradiation damage, making them potential candidates for nuclear industry applications. We explore the interactions between a mobile edge dislocation and two distinct irradiation-induced defects (Frank loops and voids) by comparing Y3-HEA and ASS. In the case of Frank loops, we observe that Y3-HEA requires a higher critical stress for the loop to unpin from the mobile dislocation. We also introduce the concept of average obstacle strength into a radiation hardening model, predicting less pronounced dislocation loop hardening in Y3-HEA compared to ASS, especially at temperatures close to operational nuclear reactor conditions (600 K). Regarding interactions between dislocations and voids, Y3-HEA demonstrates higher void shear resistance, suggesting enhanced resistance to void formation compared to ASS.

The people involved in achieving these results include Anna Fraczkiewicz, MINES Saint Etienne; Ghiath Monnet, EDF; Gilles Adjanor, EDF; Christophe Domain, EDF; Giovanni Bonny, SCK CEN. This project was funded under ANR-HERIA.

Bio: Dr. Ayobami Daniel Daramola is a research associate at the Institute for Condensed Matter and Complex Systems at the University of Edinburgh. His academic journey began with a BSc. Degree in Physics and Electronics from Adekunle Ajasin University Nigeria in 2015. Subsequently, he pursued an MSc. Degree in Theoretical Physics at Université de Cergy Pontoise in France, graduating in 2019. During his MSc. studies, he conducted research at the ESPCI-PMMH Lab in Paris, focusing on studying plasticity events in amorphous materials using a mesoscopic approach. Dr. Daramola defended his Doctorate degree in 2024 at the Ecole des MINES de Saint Etienne, specializing in Materials Science and Engineering. Currently, his research centers on developing software that generates force fields by integrating reverse Monte Carlo and Ab initio code. This software aids in accurately characterizing disordered systems such as simple liquids, liquid mixtures, and glasses obtained from diffracted experiments. His expertise lies in computational material science and soft matter physics.