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Mechanical Performance of NiFeCrMn Alloy Under Tensile Loading: An Experimental and Atomistic Model

F. Javier Dominguez[*1], M. Frelek-Kozak[1], G. Markovic[2], A. Zaborowska[1], A. Daramola[3], M. Stróżyk[1], and L. Kurpaska[1]

[1]National Centre for Nuclear Research, NOMATEN CoE, st. A. Soltana 7, 05-400 Otwock, Poland
[2]Institute for Technology of Nuclear and Other Mineral Raw Materials, 11000 Belgrade, Serbia
[3]University of Edinburgh, School of Physics and Astronomy, Edinburgh, Scotland

INTRODUCTION

- The **INNUMAT** project addresses the development of Co-free alternatives, primarily based on the CrFeMnNi system, which retains key characteristics of HEAs while exhibiting phase stability for nuclear applications.
- High-entropy alloys (HEAs) offer exceptional mechanical properties, thermal stability, and radiation resistance, making them ideal candidates for advanced nuclear systems. Co-free NiFeCrMn-based HEAs stand out due to their superior strength and ductility.
- This study combines atomistic computational modeling with experimental validation to assess the mechanical performance of NiFeCrMn HEAs under tensile loading at both room and high temperatures.

DESCRIPTION OF RESEARCH PROJECT

This study employs atomistic computational modeling validated by experimental tensile testing to investigate the mechanical performance of NiFeCrMn HEAs. Simulations include both single-crystal and polycrystalline samples, examining the effects of temperature, grain structure, and crystallographic orientation.

METHODOLOGY

- Experiments: Designed for small-scale uniaxial tensile testing at high temperature
  - Strain rate 10^{-3} s^{-1}
  - Heating rate 20 °C/min
  - EBSD images for grain boundaries and orientations
- Simulations: MD approach for uniaxial tensile test

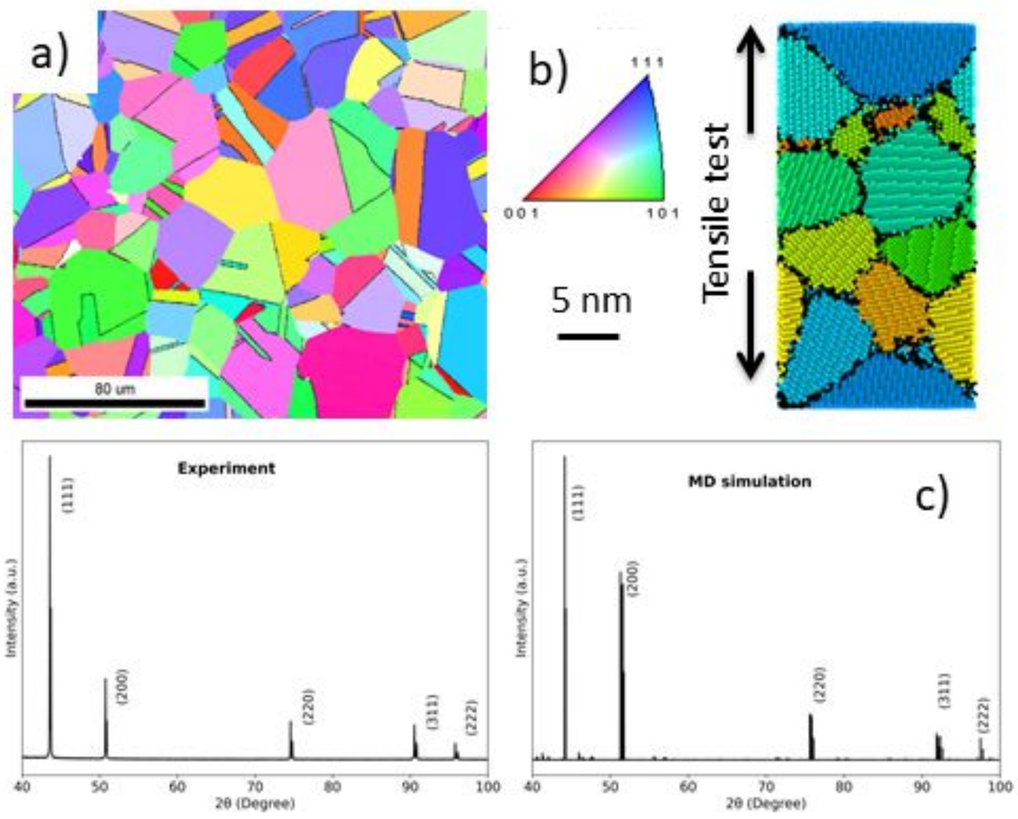

Fig 1. EBSD image of the recrystallized HEA-1 sample before tensile testing. (b) Schematic representation of the polycrystalline MD model used for tensile simulations. (c) XRD patterns of the experimental and simulated samples at room temperature, demonstrating good agreement.

RESULTS

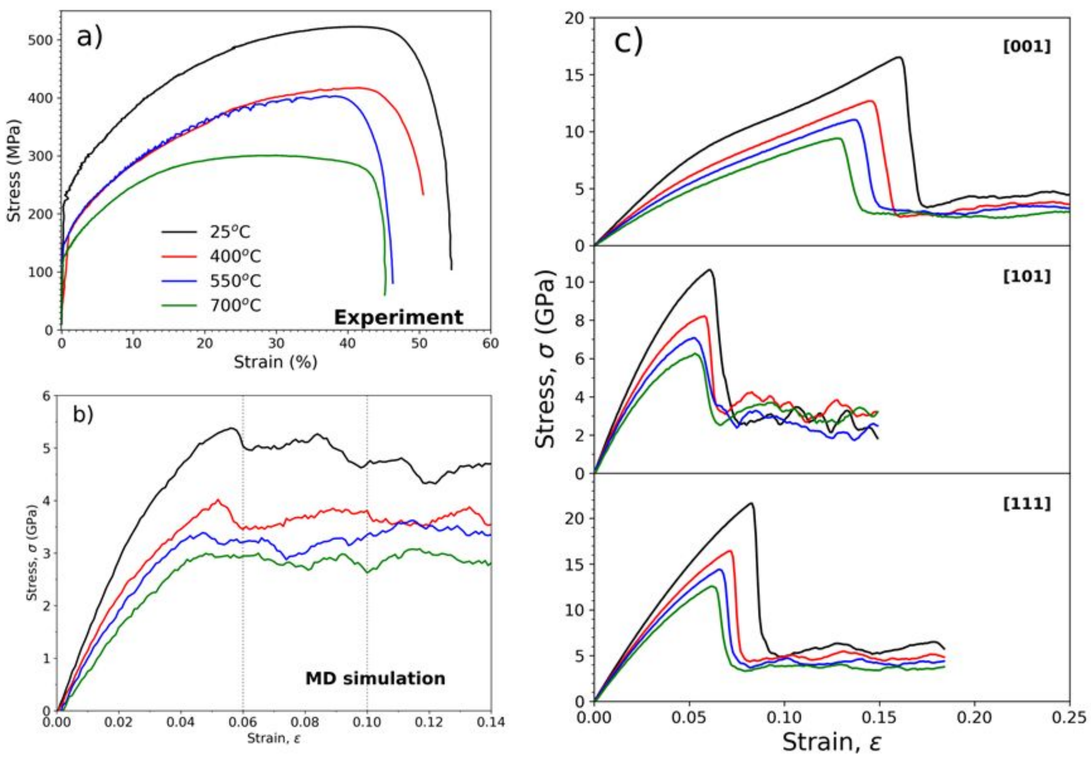

Figure 2. Stress-strain curves for polycrystal HEA-1 as a function of the temperature for experimental results in a), and MD modeling in b). While the mechanical response of single crystal grains by MD modeling is shown in c).

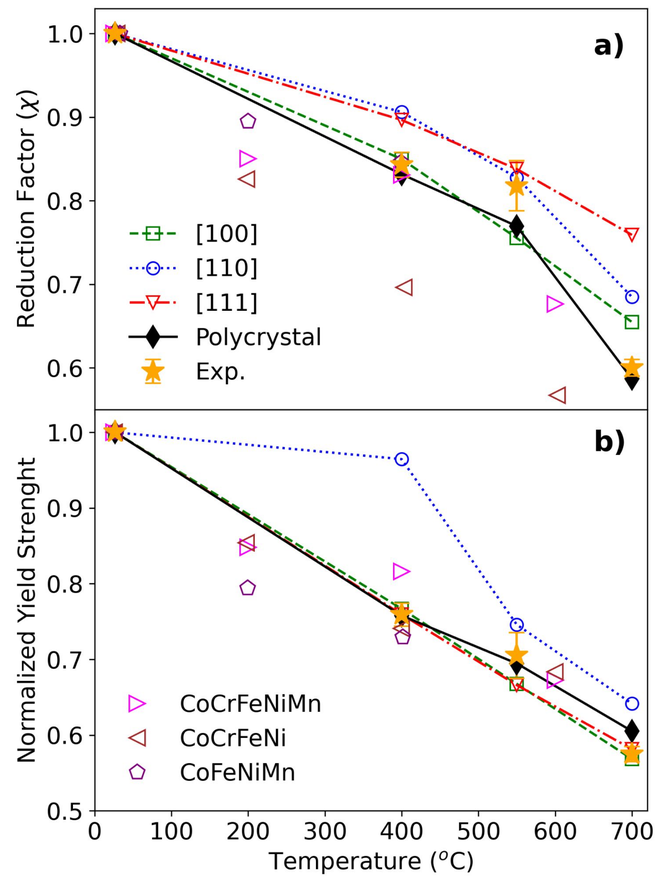

Fig 3. Experimental results and MD simulations for the reduction factor and normalized yield strength (YS). We include results for CoCrFeNi, CoFeNiMn, and Cantor alloy.

CONCLUSIONS

- The study demonstrates that the NiFeCrMn system, as a Co-free alternative, retains high strength and ductility while exhibiting distinct deformation influenced by stacking fault energetics, grain structure, and temperature effects.
- MD modeling accurately captures the mechanical behavior of NiFeCrMn HEAs, providing a reliable computational tool for predicting material performance in extreme environments, including nuclear applications.

ACKNOWLEDGEMENTS

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