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Research Assistant Position Available – Molecular Dynamics Simulation of High Entropy Alloy Coating Properties (Doctoral Student Opportunity)

The Position

Dr. Wylie Stroberg and Dr. André McDonald of the Department of Mechanical Engineering at the University of Alberta invite applications and queries for a doctoral (PhD) student position in **Molecular Dynamics Simulation of High Entropy Alloy Coating Properties**. This position will be open to candidates who possess a Master of Science degree in Mechanical Engineering, Materials Science, Engineering Physics, or related fields. Applicants with expertise and experience in materials modelling, molecular dynamics simulation, continuum mechanics, fracture and damage modelling, or thermal spraying with an emphasis on modelling are highly encouraged to apply. The successful candidate will be required to work independently and must communicate well in English. Some national and international travel may be required. The successful candidate will be financially supported. This position is available to Canadian citizens, permanent residents of Canada, refugees in Canada, and international applicants. It is expected that the successful candidate will take up the position in May, July, or September 2022. Interested candidates may wish to visit <https://stroberg-lab.github.io> to learn more about the Computational BioSystems Lab and <https://sites.ualberta.ca/~andre2/> to learn more about the Advanced Heat Transfer and Surface Technologies Laboratory.

The Project

The proposed research project seeks to design next-generation high entropy alloy (HEA) coatings with desirable mechanical characteristics using molecular dynamics (MD) simulation approaches in combination with physics-based machine learning algorithms. The outcome will be predictions of mechanical properties suitable for HEA coatings designed for extreme environments (e.g., wear and corrosion). The selected candidate will also connect predictions of microstructural features (e.g., phase formations, stacking fault energy, and dislocations) in HEA coatings to mechanical properties. The predicted models will be validated with experimental data drawn from assessments of the performance of next-generation cold-sprayed and flame-sprayed HEA coatings. Mechanical properties and performance assessments will include hardness testing and estimates of yield strength, fracture toughness, ductility, ultimate strength, and strain hardening ability. The selected candidate will make fundamental contributions to multi-scale modelling to understand the influence of microstructural and mechanical properties of HEA coatings necessary for enhancement of wear- and corrosion-resistant behavior.

Training and Professional Development Opportunity

The training of research assistants and fellows is paramount. The selected candidate will receive formal training in the following foundational and practical areas: (i) HEA materials selection and development; (ii) development of machine learning-based MD potentials; (iii) high-performance computing with massively-parallel CPU and GPU codes; (iv) visualization and analysis of large simulation datasets; (v)

multiscale modelling of materials; (vi) mechanical testing and materials characterization; (vii) surface preparation, (viii) high-quality coating fabrication via cold spraying and flame spraying, (ix) programming and operation of a 20-kg payload robot, (x) operation of industrial coating deposition systems, (xi) use of materials characterization and performance testing equipment, and (xii) safety. The successful candidate will have opportunities to participate in national and international conferences and receive exposure to the expansive professional network of Dr. Stroberg and Dr. McDonald.

Preliminary Application Procedure

Candidates are asked to submit: (i) a cover letter; (ii) a detailed curriculum vitae highlighting career achievements, areas of research, a list of publications, awards and honours, and a list of three professional references; (iii) unofficial transcripts from their undergraduate and graduate programs; and (iv) their score sheets from a test of English as a second language, if applicable.

Interested candidates should send their completed application packages and direct queries to **Dr. Wylie Stroberg** by email at **stroberg@ualberta.ca** or to **Dr. André McDonald** by email at **andre.mcdonald@ualberta.ca**.