MODELLING ISSUES FOR INNOVATIVE MATERIALS

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US Fusion Materials Science Program

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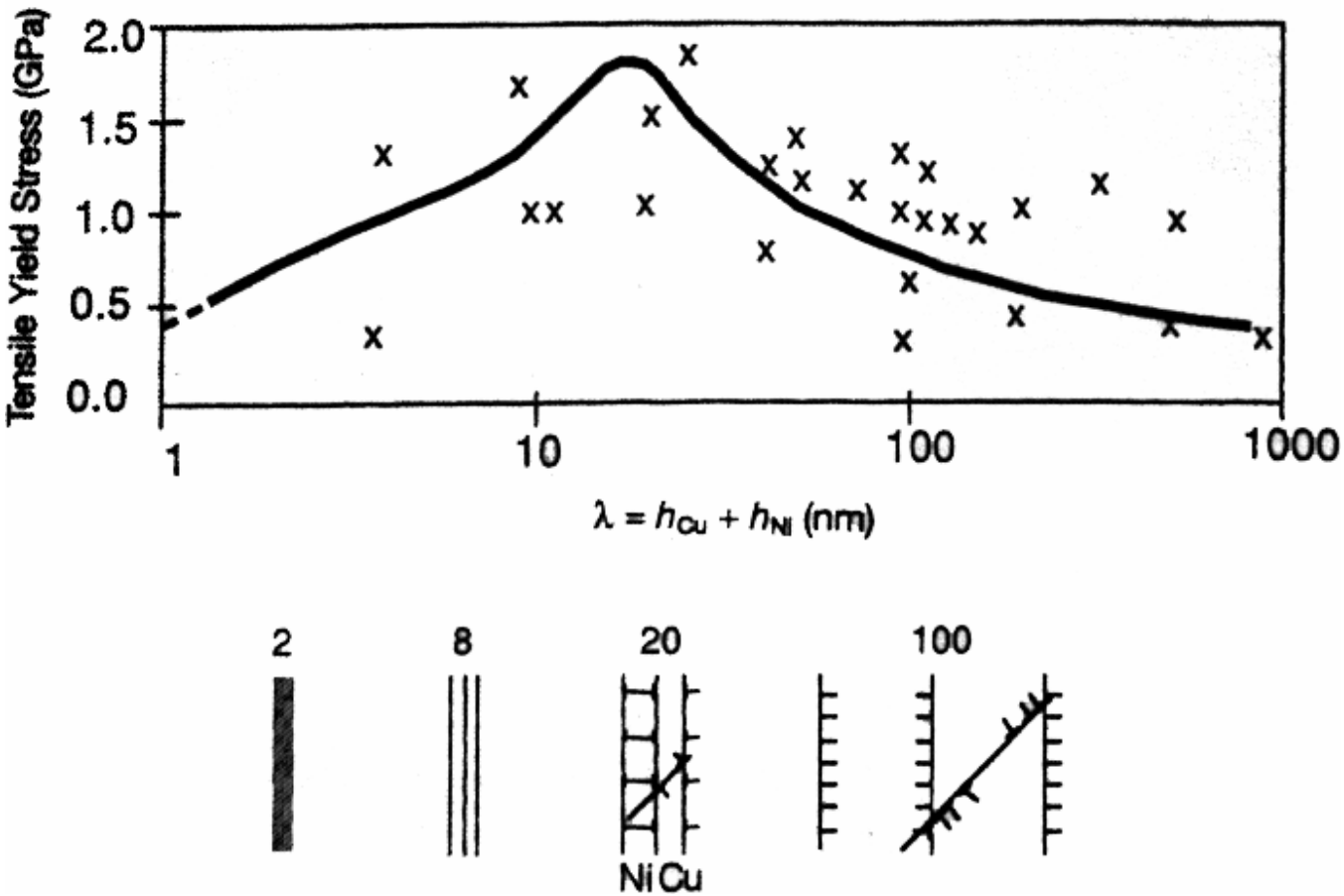
Strength of Cu-Ni Multi-layer



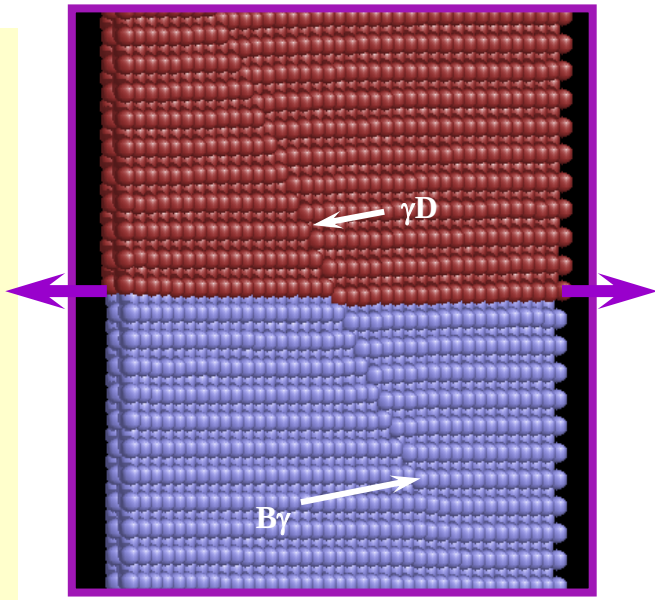
(1) Hall-Petch & Grain Size Effects

Key Issues:

- Design ultra-strong and ductile nano-scale composites.
- Determine the relationship between processing methods and strength/ ductility;
- Design factors for strength:
  - Strain in epitaxial layer;
  - Elastic moduli;
  - Slip geometry
  - Interfacial Dislocation Network;
  - Nano-size precipitates;
  - Radiation-induced Microstructure (SIAs, SFTs) near interfaces;

(2) Interface Resistance to Deformation

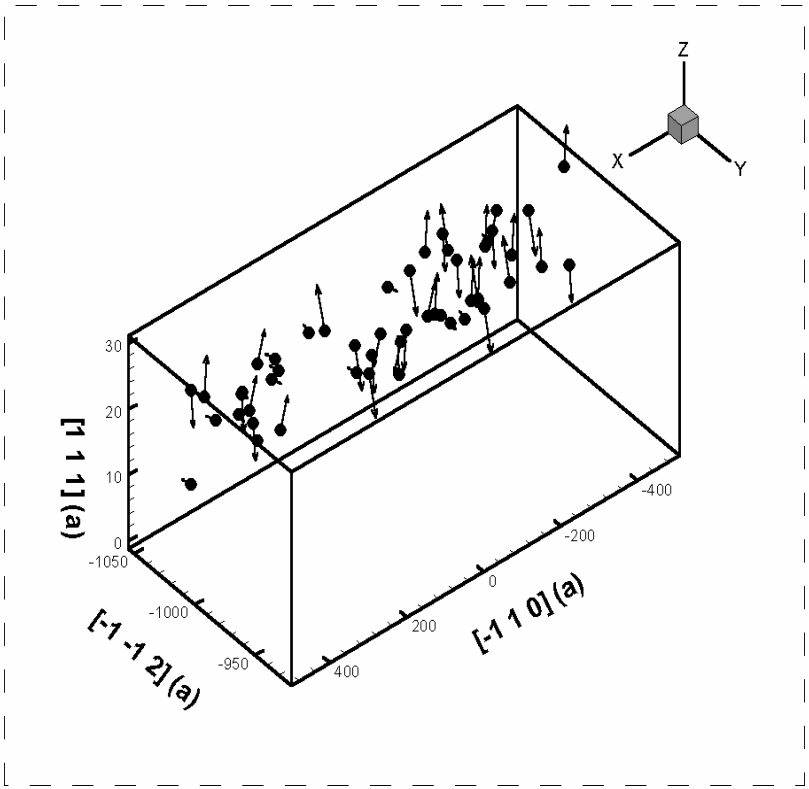
- Ab-initio and MD simulations of dislocation core spreading, Peierl's stress and mobility across interfaces;
- Control and Stability of Confined Layer Slip (CLS) in Small Volumes;
- Effects of Radiation Mixing on Deformation;
- Co-deformation of incompatible slip systems (e.g. FCC/BCC).

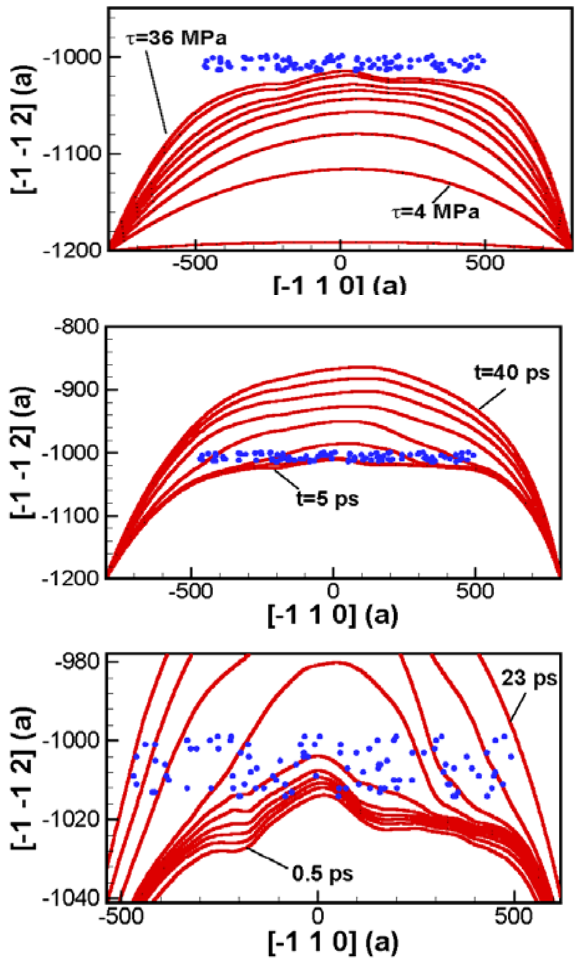


(3) Radiation Stability of Nano-precipitates

- Cascade-Precipitate Interaction;
- KMC simulations for the dissolution kinetics of nano-scale precipitates;
- Kinetic/ Thermodynamic Modeling of Nano-precipitate evolution and chemistry under irradiation;
- Helium bubble formation at nano-precipitates;
- Sink efficiency of nano-precipitate interfaces;
- SIA – nano-ppt interaction;

(4) Plastic Instabilities in Ultra-strong Materials





(5) Radiation Mixing of Nano-scale Interfaces

- MD modeling of cascade evolution across interfaces;
- Ballistic versus thermodynamic-driven interface mixing;
- Impurity, SIA cluster and void segregation;
- Compositional fluctuations in irradiated multilayer systems.