Multiscale Modeling of Space Materials

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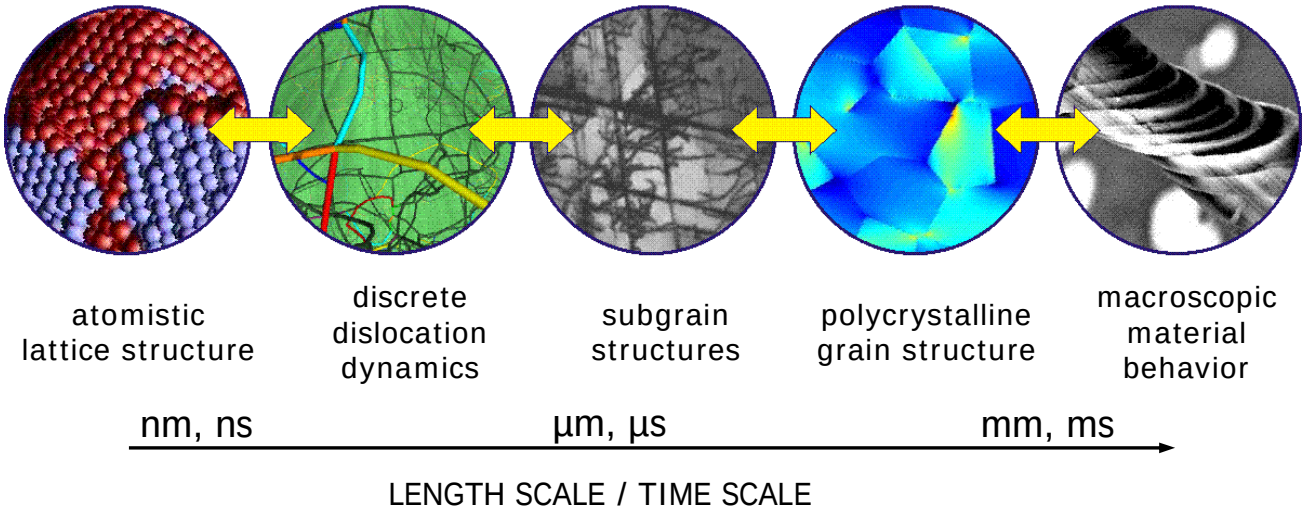
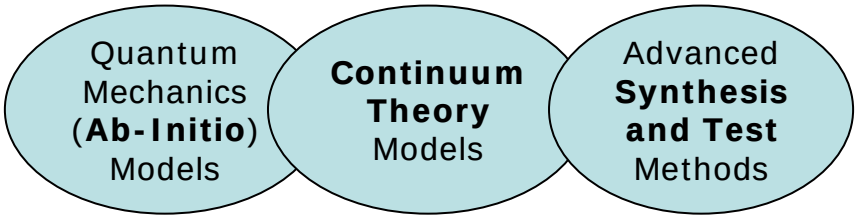


Atomistic to Continuum Models
MODEL → TEST → DESIGN

Approach



Materials of interest

- **Novel materials** operating under **extreme conditions**
- Multifunctional materials (**MESM**)
- Metal oxidation; Combustion
- Gas-metal surface phenomena

Research goal

→ **predict** the mechanical behavior of engineering materials;
design **novel materials** with exceptional performance

→ **improve** already existing materials:
metals, metal alloys and composites with nano reinforcements (i.e. CNT)

Computing: *Bulgarian GRID Portal*

- **Clusters at BAS (** 9 grid-clusters, CERN initiative)
  - **Madara cluster at IICT*, IOCCP****
    Linux based system
    102x4 microprocessors (Intel XEON HyperThreading E5520)
    Location: Supercomputing Center of the IOCCP-BAS**

- **IBM Blue Gene/P super computer** (since 2008)
  Linux based system :
  8192 microprocessors: 23.42 trillion operations per sec (TFLOPS)
  Location: Supercomputing Center of the SAITC***

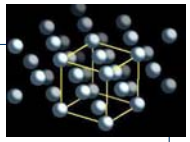
BG08-MADARA
Grid Cluster

Physical CPU	800
Logical CPU	800
Spec CPU 2006	21440
SI2K	1600
Storage	24 TB
Location	IOCCP-BAS

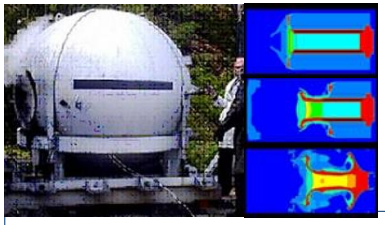
* IICT – Institute of Information and Communication Technology
** IOCCP – Institute of Organic Chemistry with Center of Phyto Chemistry
*** SAITC – Bulgarian State Agency for Information Technology and Communications

Novel materials, Development

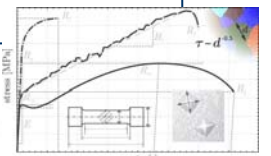
Material Tests and
Model Validation Tests

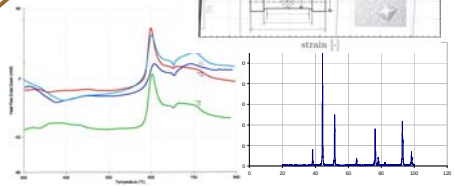


Multiscale Modeling:
- *First-Principles,* MD, Meso scales and continuum scale models.
- Constitutive Equations, dual branches of Failure criteria
- Bridging scales to continuum



Critical experiments to validate constitutive equations, strength, toughness, reaction Initiation, and Reaction propagation



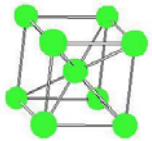


- Synthesis
- Binder + Gas phase materials
- Reinforcement
- Fracture characteristics and improvement of fracture toughness

APPLICATIONS
Design, Analysis to replace Conventional materials with Advanced function materials; demonstration of an application; Hybrid Designs

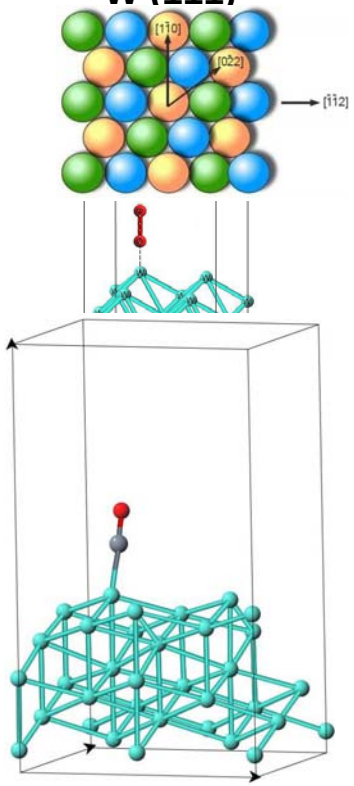
Ab-Initio Chemical Reaction Models

Metal – Gas



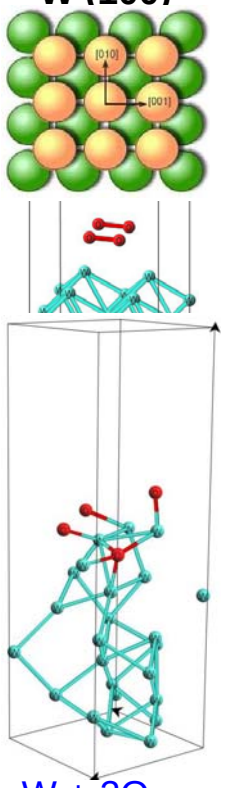
W (bcc), #74: [Xe] $4f^{14}\ 5d^4\ 6s^2$

W (111)



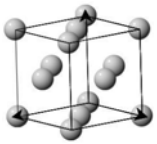
W + CO
0 K
“ontop” site

W (100)



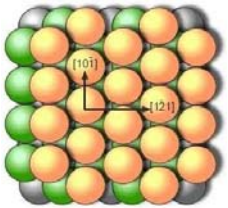
W + $2O_2$
950 K
“lying down”

Metal – Metal

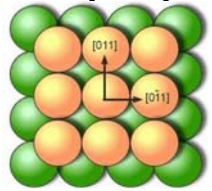


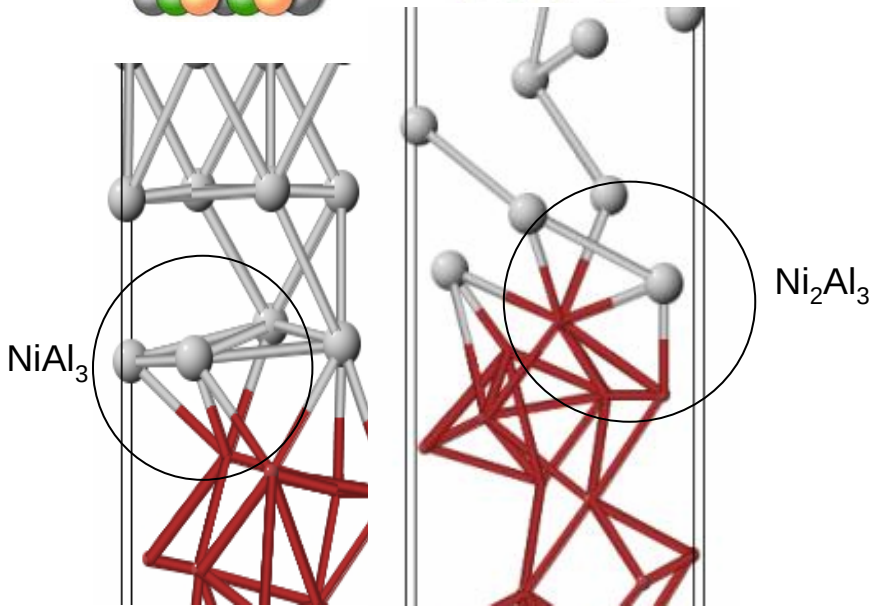
Al (fcc), #13: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$
Ni (fcc), #28: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2 3d^8$

Ni (111)



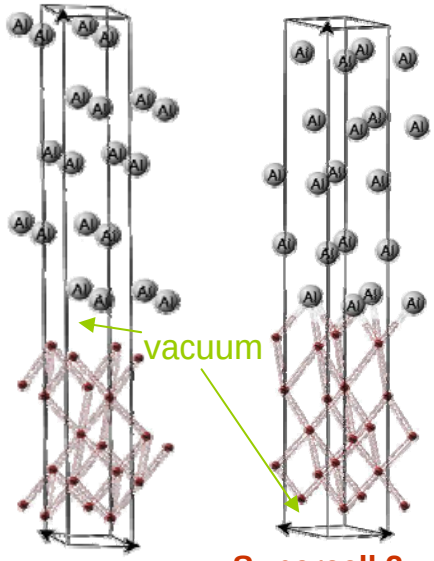
Ni (100)





Ni + Al mixture, 660 C

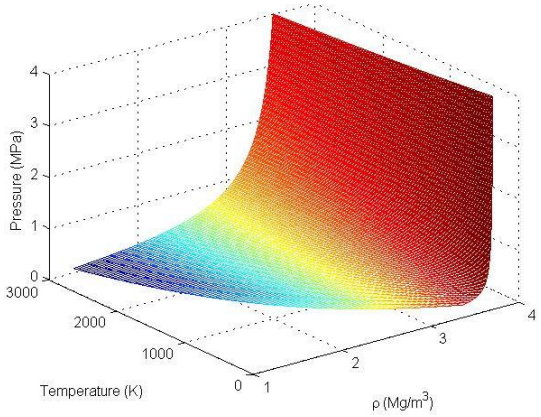
MESM, Equation of State

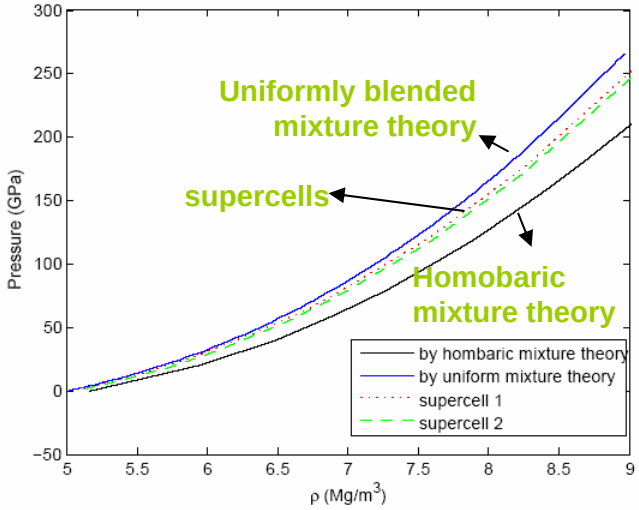


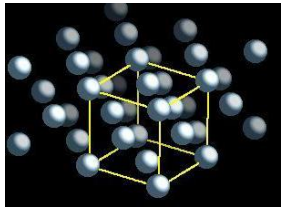
Supercell 1 Supercell 2

By Mixture Theories
By Supercell Approach

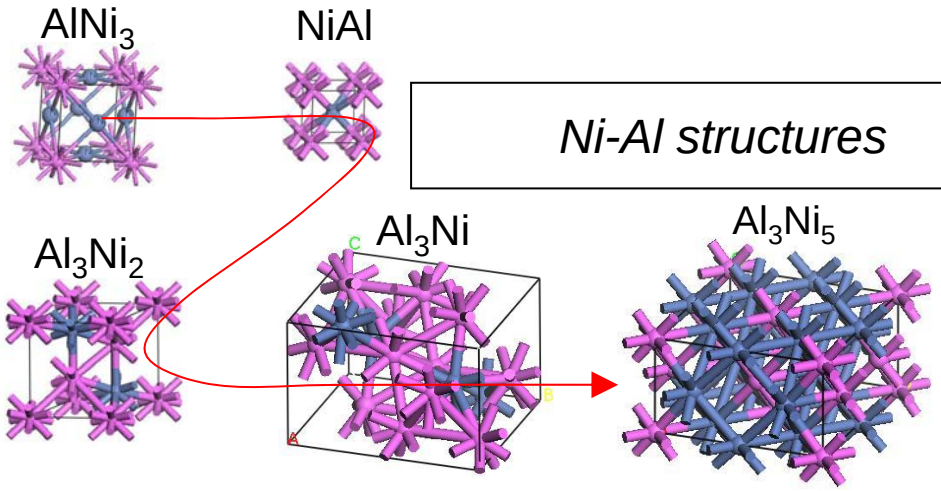
EOS of 3Al+Ni+15%porosity MESM





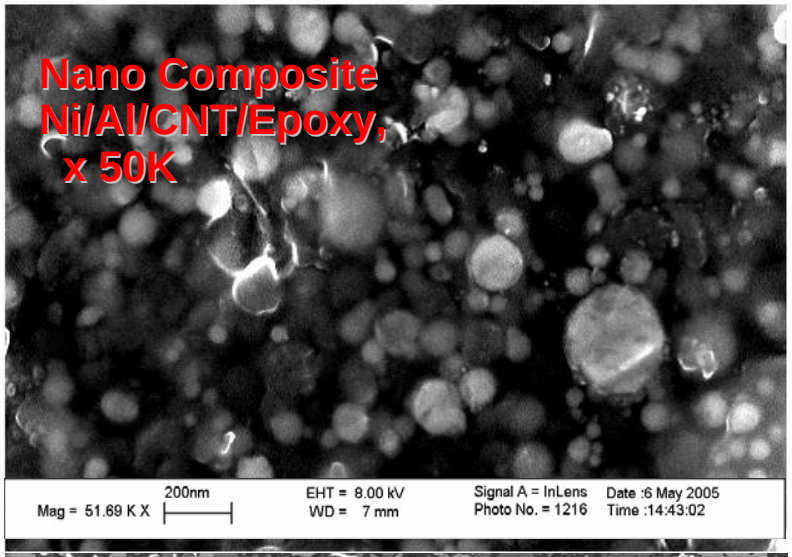


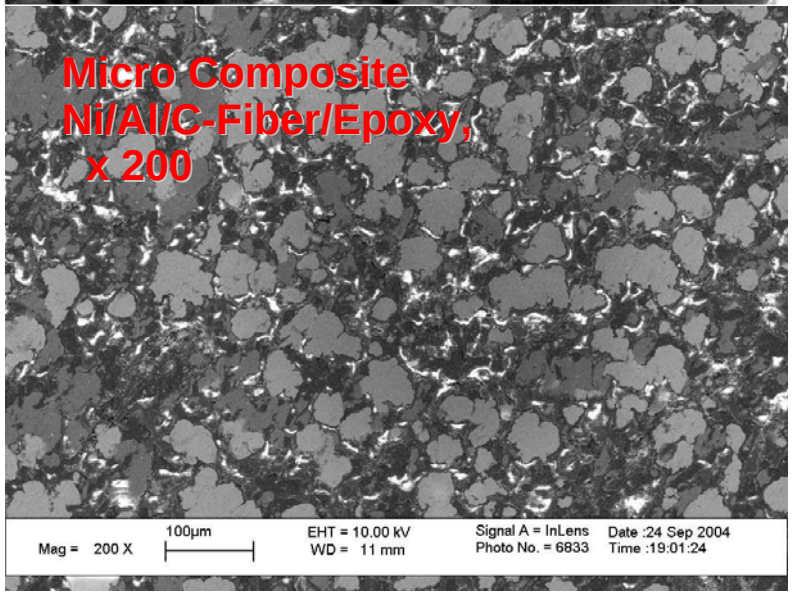
Al, Ni (fcc)



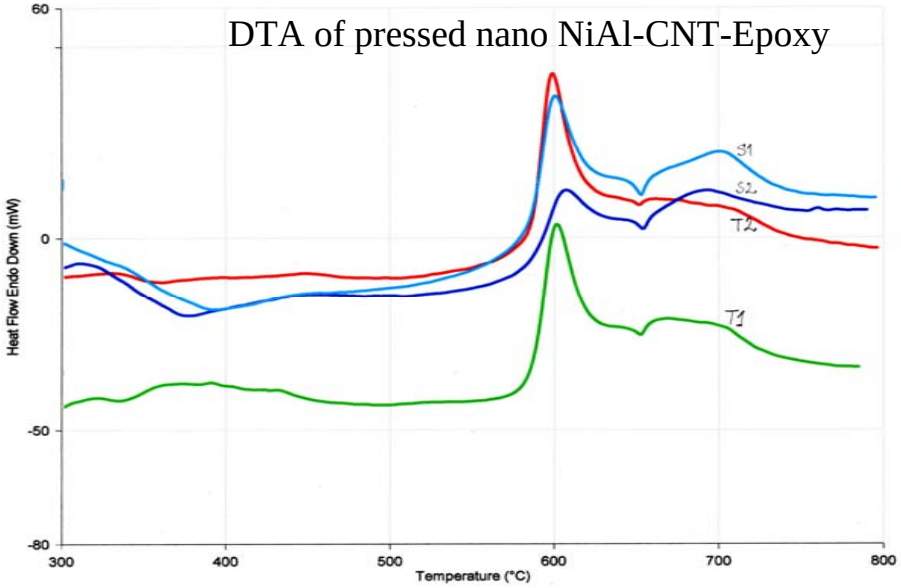
Characterization

SEM of pressed nano and micron powder samples





DTA of pressed nano NiAl-CNT-Epoxy



XRD of pressed nano NiAl-CNT-Epoxy