Barend Thijsse

Professor - Principal Investigator

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Research interests
Selected materials interface properties, studied by atomic-scale computational modeling: adhesion, plasticity, oxidation, phase transformations, extreme nonequilibrium, nanomechanics. Metals, semiconductors, oxides, polymers, liquids.

Atomistic Modeling at Interfaces

Recent Research activities
-Pilot project on Force-biased Monte Carlo mixed with Molecular Dynamics
-Improvement of spline fitting algorithm
-Improvement of crystal type assignment and visualization to atoms
-Purchase of GPU-computer
-Pilot project on truly tunable materials

===Contributions to joint research===
TUD-3mE (Prof. Dik) -- Materials analysis in art
TUD-Civil Engineering (Dr. Simone) -- Structural batteries, Fiber-polymer composites
TUD-Nanoscience (Prof. Kouwenhoven, Prof. Bakkers) -- Supeconductor thin coating deposition
TUD-Nanoscience (Prof. Steeneken) -- hexagonal BN
TUD-Nanoscience (Prof. Caviglia) -- Perovskite interfaces
DIFFER (Dr. Klaver) Helium in tungsten
SKF (Dr. Echeverri) -- Lubrication
NIST Washington DC (Dr. Rust) -- Supernova luminosity analysis
Various partners -- Seawater desalination

Key publications 2015
Rust, B.W., Pruzhinskaya, MV & Thijsse, BJ, *Calibrating the decline rate: Peak luminosity relation for type Ia supernovae,*
Meeting Abstracts of the XXIX IAU General Assembly Meeting, 2015.

Srinivasan, P, Nicola, L, Thijsse, BJ & Simone, A *Molecular dynamics simulations of the two-way shape-memory effect in NiTi nanowires,*
Proceedings Symposium P: Nanogenerators and Piezotronics Vol. 1782. MRS Symposium Proceedings (pp. 35-40), 2015.

Andrew Ian Duff, M.W. Finnis, Philippe Maugis, Barend J. Thijsse, and Marcel H.F. Sluiter, *MEAMfit: A reference-free modified embedded atom method (RF-MEAM) energy and force-fitting code,*
Comput. Phys. Com. 196 (2015) 439-445.

Daniele Scopece and Barend J. Thijsse, *Comment on: "An improved molecular dynamics potential for the Al-O system" Comput. Mater. Sci. 53, 483 (2012),*
Comput. Mater. Sci. 104 (2015) 143-146.

Fidel Valega Mackenzie and Barend J. Thijsse, *Study of metal/epoxy interfaces between epoxy precursors and metal surfaces using a newly developed reactive force field for alumina-amine adhesion,*
J. Phys. Chem. C 119 (2015) 4796-4804.

Other Achievements
Architect of new departmental structure

Split-up of section Virtual Materials & Mechanics section into three computational groups
AMI group: Focus shift to interfaces between dissimilar materials

Graduate School student coach, teacher, mentor