



**HAL**  
open science

## Elastic and piezoelectric properties of nanowires: from atoms to continuum, from chemistry to mechanics

Gilberte Chambaud, Alexander Mitrushchenkov, Julien Yvonnet

### ► To cite this version:

Gilberte Chambaud, Alexander Mitrushchenkov, Julien Yvonnet. Elastic and piezoelectric properties of nanowires: from atoms to continuum, from chemistry to mechanics. Recent advances in Material Science” CCS-SCF meeting, Oct 2013, Paris, France. hal-01081755

**HAL Id: hal-01081755**

**<https://hal.science/hal-01081755>**

Submitted on 10 Nov 2014

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# **Elastic and piezoelectric properties of nanowires: from atoms to continuum, from chemistry to mechanics**

**Gilberte Chambaud**

Laboratoire Modélisation, Simulation Multi-Echelle, MSME  
UMR 8208 CNRS - Université Paris-Est Marne la Vallée,  
5 bd Descartes, 77454 Marne-la-Vallée, France

## **Abstract**

Experimentally, mechanical and piezoelectrical properties of individual nanowires have been extensively explored. However, predicting properties of structures or composites based on electromechanic nanowires is highly challenging and remains an open problem for the following reasons: (a) the multiscale nature of the problem: the response of the composite is macroscopic, while the structure is defined at the nanoscale level, and the properties of the constituents, as well as the interactions (interfaces mechanics) between the constituents must be predicted at the atomic scale. Furthermore, determining the different coefficients associated with the properties at the nano/atomic level requires *ab initio* quantum mechanics calculations; (b) electromechanical models for continuum mechanics describing surface effects due to the nanoscale have not been proposed so far; (c) the computational costs can be out of scope if we do not introduce appropriate couplings between scales and models to take maximum advantage of each model in its range of validity. Thus, multiscale modelling strategies as well as novel numerical methods seem the only way to fully describe electromechanical nanowire-based composites.

Starting from fully atomistic calculations, we have developed a classical, continuous mechanics, model of wurtzite nanowires, using FEM discretization. *Ab initio* calculations of AlN and ZnO wurtzite [0001] nanowires have been performed with diameters up to 4 nm. It is shown that the nanowires can be well represented by an internal part with AlN bulk elastic properties, and one-atomic surface layer with its own elastic behaviour. To deal with more nanostructures/nanoparticles complex geometries, a finite element method using surface elements with their own elastic properties is developed. The surface elastic coefficients are provided by *ab initio* calculations through a slab procedure. The finite element model is compared with the full *ab initio* nanowires calculations and a good agreement is demonstrated.