

## Atomic structure relaxation in NiO nanoparticles studied by x-ray absorption spectroscopy in combination with molecular dynamics

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In this study we present the results of nanocrystalline NiO investigations using the Ni *K*-edge extended x-ray absorption fine structure (EXAFS) [1] and recently developed modelling technique, combining classical molecular dynamics (MD) with *ab initio* multiple-scattering EXAFS calculations (MD-EXAFS) [2].

Conventional analysis of the EXAFS signals from the first two coordination shells of nickel revealed that (i) the second shell average distance  $R(\text{Ni}-\text{Ni}_2)$  expands in nanocrystalline NiO compared to microcrystalline NiO, in agreement with overall unit cell volume expansion observed by x-ray diffraction [3]; (ii) on the contrary, the first shell average distance  $R(\text{Ni}-\text{O}_1)$  in nanocrystalline NiO shrinks compared to microcrystalline NiO; (iii) the thermal disorder contribution into the mean-square relative displacement (MSRD)  $\sigma^2$  is close in both microcrystalline and nanocrystalline NiO and can be described by the Debye model; (iv) the static disorder is additionally present in nanocrystalline NiO in both the first Ni–O<sub>1</sub> and second Ni–Ni<sub>2</sub> shells due to nanocrystal structure relaxation. Within the MD-EXAFS method, the force-field potential models have been developed for nanosized NiO (Fig. 1) using as a criterion the agreement between the experimental and theoretical EXAFS spectra, revealing the role of the nickel vacancies and size of the nanoparticle [3,4].

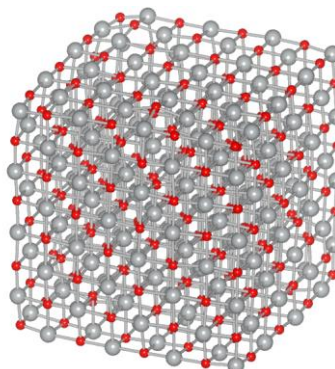


Fig. 1. NiO nanoparticle model.

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### References

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