Direct measurement of Ni incorporation into Fe_3O_4(001)

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The iron oxides are the archetypal cation defect material. For magnetite (Fe_3O_4) these cation vacancies can play an important role in its surface chemistries. Specifically, Fe_3O_4 has been observed to pattern the adsorption of a wide range of metal adatoms onto its (001) surface, including those of the catalytically interesting platinum group metals (PGMs). The metal adatoms occupy a projected bulk tetrahedral site where two sub-surface octahedral vacancies and one surface tetrahedral interstitial kinetically hinder the sintering of the metal adatoms into nanoparticles.

Despite this, STM observations of several first row transition metals, e.g. Ni and Co, suggest that these adatoms can be thermally driven into the subsurface octahedral vacancies [1]. Here we present an X-ray standing wave (XSW) study directly demonstrating the co-existence of Ni in a surface tetrahedral site, a subsurface octahedral site and a bulk octahedral site confirming the interpretation of previous STM measurements and quantitatively probing the vertical displacement of the Ni atoms at each location.

References:
[1] R. Bliem, et al. Phys. Rev. B, **92** (2015) 075440