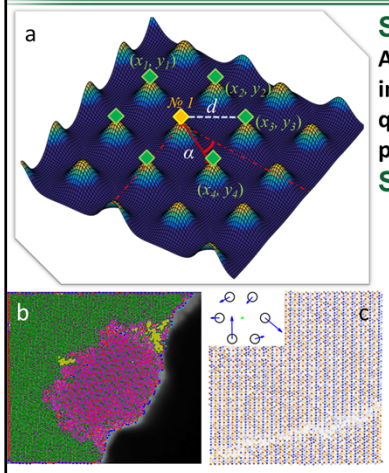
Identification of phases, symmetries, and defects through local crystallography



(a) Central atom and 6 neighbors with distance and angle metric assignments shown; (b) Mo-V-Te-Ta oxide surface atom clustering reveals multiple obvious and novel phases; (c) Mo-V-Te-Ta oxide with a hidden lattice shift revealed only by the algorithm.

Work was performed at Center for Nanophase Materials Science

Scientific Achievement

An entirely new approach based on statistical analysis of individual atomic neighborhoods allows an in depth, quantitative description and identification of chemical and physical phase information at all captured length scales.

Significance and Impact

We recover information in high resolution imaging that goes far beyond visual analysis, and includes scale independent, quantitatively mapped, feature, structure and chemical behavior recognition.

Details

- Atoms and their neighbors reveal preferential structures and symmetries that dictate global chemistry
- Our algorithm explores any sized local atomic positions agglomerates to reveal, identify, and classify tiny structural distortions
- Chemical data analysis in imaging becomes automatable, quantitative, searchable, and scalable

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Feature based statistical analysis of atomically resolved images reveals the connectivity of lattice and bond structure, as well as highlights structural distortions, thus allowing for quantitative chemical description and identification of phases. High resolution atomic scale images are costly to obtain as well as difficult and time consuming to analyze; we pave the way for automatic, full information recovery from high resolution imaging such as electron and scanning probe microscopies that allows for classification and automatic identification of materials that is fully scalable to practically any number of images and features, and executes on the order of seconds. Unlike the classical, symmetry based descriptions, our approach utilizes local characteristics of the immediate atomic environment, the size of which is user defined, like the structure of the local atomic neighborhood and the type of bonding. This statistical description illustrates the predominant, statistically significant, distortions and ranks them in terms of relevant prevalence. This type of information allows scientists to see beyond the image and extract behavior typically that typically cannot be seen, like the number of atoms in various automatically identified phases of the catalytic compound shown, Mo-V-Te-Ta oxide, phase uniformity, and interface interactions.

Reference

"Identification of phases, symmetries and defects through local crystallography"

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