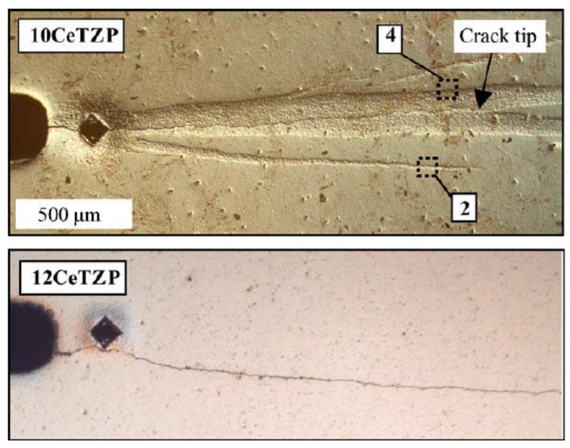
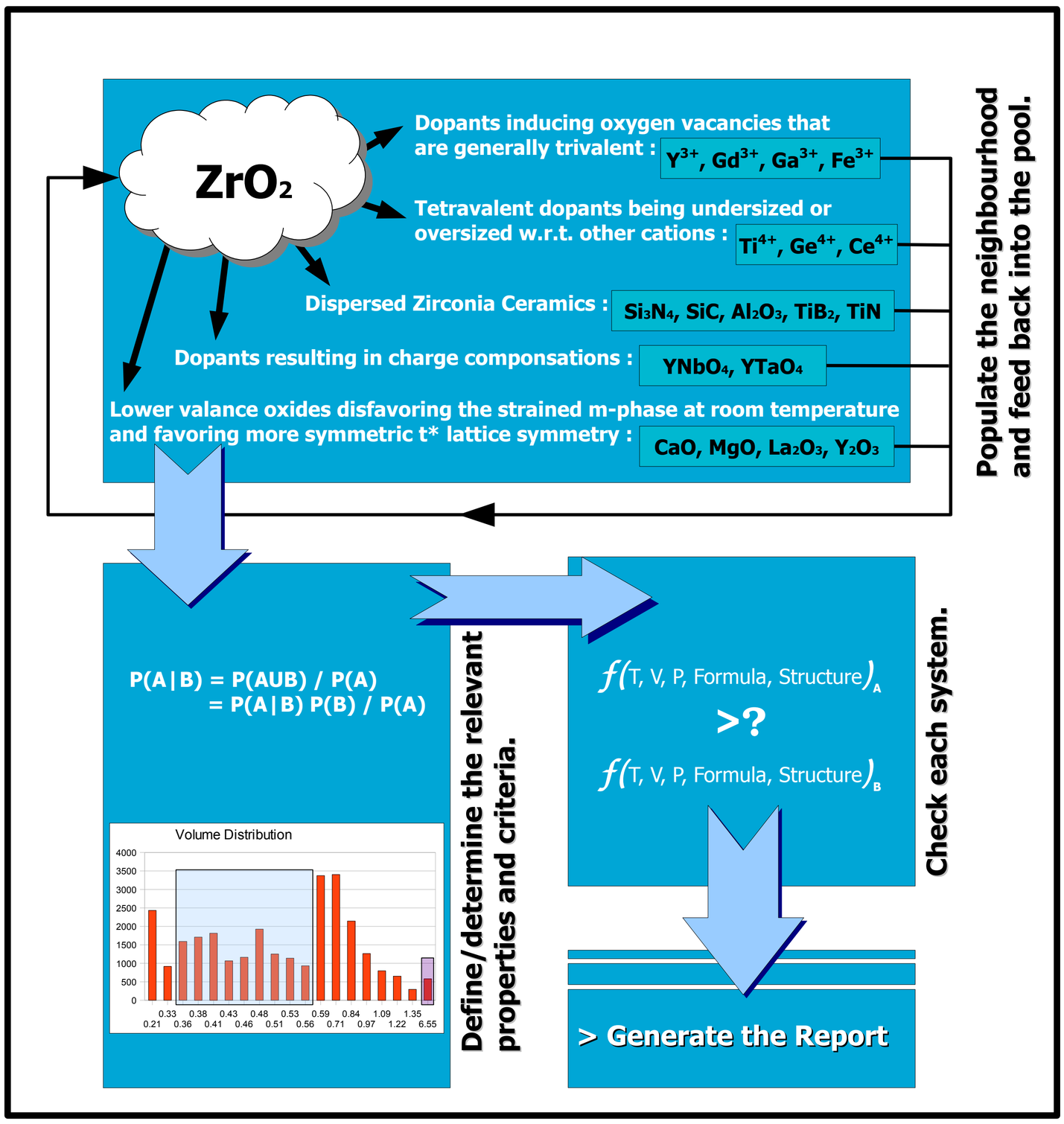


Self Healing Mechanism vs. Cracks

Transformation toughening mechanism observed in ZrO_2 is due to the extraordinary ability of the zirconia to expand in volume when undergoing a phase transition from a higher symmetry structure (tP6) at high temperature to a lower one (mP12) at ambient temperature. The accompanying volume increase is about 4% and this transition attacks the crack propagation from various angles: it uses the propagation's energy for the trigger mechanism; the expansion pushes the surrounding volume causing a shift towards the crack hence closing the crack in the wake and further consumes the crack propagation energy via scattering.

Materials Informatics for Transformation Toughening

Emre S. Tasci, Marcel H.F. Sluiter



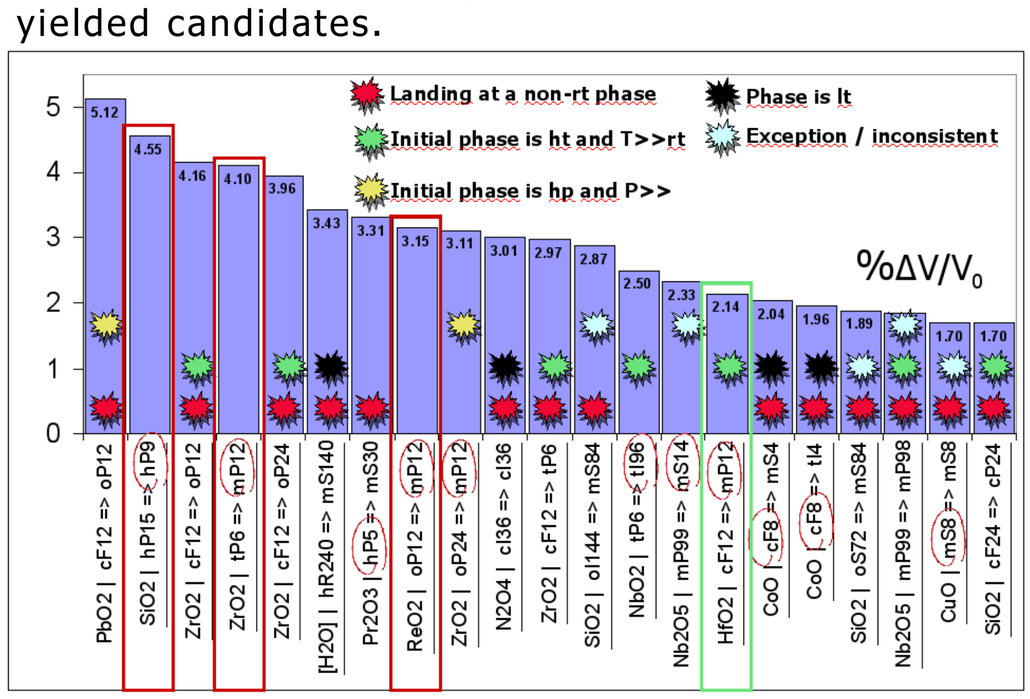
Algorithm Representation
Even when there is scarcity in data, clustering via similarity relations creates a pool of candidates for investigations. The filtering criteria can use any external modules as well as the internal ones via a scoring system.

Zirconia, a material known for its transformation toughening property is also renown for its applications in the jewelry sector which makes it an expensive component for the self healing ceramics.

This project aims to find candidate materials that also possess the ability through the use of materials informatics employing data-mining, clustering and informatics methods. For this purpose, materials databases (DBs) were constructed and relations /protocols between them were defined/implemented by developing software tools and interfaces.

Currently, the structure DB contains about 160000 structural entries on multinaries and it is based on the Linus Pauling File. There are also the physical properties DB (42000 entries) and the referential DBs such as the crystallography DB and the elemental DB.

The system was first run using the binaries DB containing about 28000 structural and 17000 physical property entries. Even with this limitation and the additional handicap of doing the reckoning in the extensively explored region of binaries, the search yielded candidates.



Binary search results for transformation toughening materials
Covers not only the materials in standard conditions but also high temperature and pressure cases.

Ends here?

Since the materials databases have been constructed now and the analysis tools having been developed, the flexible applicability of the informatics allows for various other searches by merely redefining the similarity relations and filtering criteria.

References

- Villars P., Onodera N., Iwata S. *J. Alloy Compd* **279** 1 1998.
- Deville S., El Attoui H., Chevalier *J Eur Ceram Soc* **25** 3089 2005.

Emre S. Tasci, Marcel H.F. Sluiter

Structure & Change in Materials
Department of Materials Science & Engineering
3mE / TUDelft 2628 CD Delft

e.tasci@tudelft.nl

DCMat Delft Centre for Materials

Virtual Materials Laboratory

TU Delft Delft University of Technology

Challenge the future