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## High temperature phase transformation and the mechanism in YTaO<sub>4</sub>

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High temperature phase transformation and the mechanism in  $YTaO_4$  ceramics as potential thermal barrier coatings material is investigated by experiments and first principles calculation. High temperature *in situ* XRD and Raman were indentified the phase transformation of yttrium tantalate. HRTEM showed the microstructure of phase transformation between monoclinic phase and tetragonal phase. The mechanism of phase transformation was discussed by the first principles calculation combined the Landau free energy expansion. Calculations of Gibbs free energies show that the phase transformation temperature at 1430°C, close to the experimental value of  $1426\pm7^{\circ}$ C. Landau free energy expansions demonstrate that the transition is second order and, based on the fitting to experimental and calculated lattice parameters, it is found that the transition is a proper rather than a pseudoproper type. Together, these finding are consistent with the transition being ferroelastic.

## **Biography**

Jing Feng has completed his PhD in Materials Science from Kunning University of Science and Technolgy & Tsinghua University in China. He is a Postdoc Fellow and Research Associate in Harvard University at 2012-2015. He is the Director of Lab of Advanced Materials in Designing and Application of Kunning University of Science and Technolgy. He has published more than 100 papers in reputed journals and has been cited more than 1000 times.

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