Contribution ID: **226** Type: **Poster Presentation**

Computational study of some tin dioxide phases.

Wednesday, 13 July 2011 17:00 (2 hours)

<p>Rutile and anatase structured tin dioxide ceramics have been intensively studied in recent years because of their potential in sensing and fuel cells. The present work uses classical molecular dynamics simulations focused on the structure and possible transformation from anatase to rutile tin dioxide. The empirical Buckingham potential has been used to describe the interatomic interactions in tin dioxide. The total energy of the NVE ensemble of the two structures at various temperatures has been calculated in order to determine the transition temperature and pressure. The results obtained showed an energy increase with temperature which was constantly compared with experiments. The radial distribution functions for the two structures suggest the transformations at temperature above 900 °C in agreement with the experiments.

Level (Hons, MSc,
   PhD, other)?

other

Consider for a student
   award (Yes / No)?

No

Would you like to <br> submit a short paper <br> for the Conference
 Proceedings (Yes / No)?

Yes

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