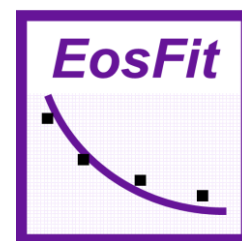




EosFit Workshop

at
ECM-2015 in Rovinj
ecm29.ecanews.org

Friday August 28th 2015
Hotel Park, Rovinj, Croatia



Description

An equation of state (EoS) describes how the volume or density of a material varies with changes in pressure and temperature. It also defines how some of the elastic properties of the material change in response to compression and expansion. Equations of state therefore provide not only fundamental thermodynamic data but also give insights in to the details of interatomic interactions within the solid state, as it is these that resist the externally-applied compressive stresses. EoS are thus fundamental to understanding the structure-property relationships in crystalline materials. Workshop participants will be introduced to equations of state to describe the volume variation of crystals with pressure and temperature, and taught how to use the EosFit-7 software to determine elastic parameters from diffraction data.

Organisers

- Dr. Ross J. Angel, University of Padova, rossjohn.angel@unipd.it
- Dr. Tiziana Boffa-Ballaran, Bayreuth, tiziana.boffa-ballaran@uni-bayreuth.de
- Dr. Matteo Alvaro, University of Padova, matteo.alvaro@gmail.com
- Dr. Daria Pasqual, University of Padova, daria.pasqual@unipd.it

Workshop Program

The workshop will open with lectures to briefly introduce the theory behind the elastic response of crystals to pressure and the concepts behind equations of state (EoS). The EosFit program (Angel et al., 2014) will be demonstrated and the participants will be guided through several worked examples on their own computers. The afternoon will be devoted to advanced topics, and to showing participants how to analyse their own high-pressure and/or high-temperature data. Participants are expected to have a good knowledge of basic diffraction theory and crystallography. No previous knowledge of EoS will be required, although participants will gain more from the workshop if they have collected their own data, or plan to do so in the near future. Participants are strongly encouraged to bring their own datasets, especially problem datasets, for analysis and discussion.

Angel R.J., Gonzalez-Platas J. & Alvaro M., 2014. EosFit-7c and a Fortran module (library) for equation of state calculations. *Zeitschrift Fur Kristallographie* **229**, 405-419. Download the EosFit program from www.rossangel.net

Registration

Participation in the EosFit workshop is only possible by registering for the ECM at: <http://ecm29.ecanews.org/participate/registration/>

A reduced workshop registration fee of 30 euro has been made possible through the support of our commercial sponsors.

