Programme and Book of Abstracts

Fifth Meeting of the Italian (AIC) and Spanish Crystallographic (GE3C) Associations (MISCA V)

Napoli, 4-7 September 2019

MISCA2019

Summary

Committees…….....3

Sponsor……4

Conference Schedule…….....5

Abstracts

Plenary lectures…..…….....11

Awards…….……...14

Commercial presentations……..23

MS1 - Crystallography out of Academia…….....27

MS2 - In situ and in operando studies of systems structural evolution……...…31

MS3 - Coordination compounds to coordination materials……...…..37

MS4 - Crystal growth: from fundamentals to applications in nature and technology……..…….44

MS5 - Bio-crystallography: from Structure to Function…….……51

MS6 - Mineral structures and mineral characterization……..…58

MS7 - Crystal forms in Pharma…….…..…66

MS8 - Contemporary challenges in Structural Biology……..…73

Posters of Session 1: MS1 – MS4…….....…….…79

Posters of Session 2: MS5 – MS8…….……..….99

Committees

Steering Committee

G. Diego Gatta
AIC President
Univ. Milano

Fernando Lahoz
Past GE3C President
CSIC, Zaragoza

Organizing Committee

Luigi Vitagliano
IBB-CNR, Napoli, Chair

Michele Saviano
IC-CNR, Bari, Chair

Filomena Sica
Univ. Federico II, Napoli

Piergiulio Cappelletti
Univ. Federico II, Napoli

Consiglia Tedesco
Univ. Salerno

Luciana Esposito
IBB-CNR, Napoli

Rita Berisio
IBB-CNR, Napoli

Luca De Luca
IBB-CNR, Napoli

Alessia Ruggiero
IBB-CNR, Napoli

Nicole Balasco
IBB-CNR, Napoli

Annalisa Guerri
Univ. Firenze

Simona Galli
Univ. Insubria

Scientific Committee

Matteo Alvaro
Univ. Pavia

Giuseppe Falini
Univ. Bologna

Felipe Gándara
CSIC, Madrid

Pilar García Orduña
CSIC, Zaragoza

Andrea Ilari
IBPM-CNR, Roma

Sol López-Andres
Univ. Complutense, Madrid

Lucia Maini
Univ. Bologna

Alfonso Martínez de la Cruz
CICBioGUNE, Bilbao

Paolo Pio Mazzeo
Univ. Parma

Marta E.G. Mosquera
Univ. Alcalá de Henares

MS6 - O5: Thermodynamics, elasticity and phase stability of grossite ($CaAl_4O_7$) at high pressure and temperature

Donato Belmonte,[a] Fernando Cámara,[b] Paolo Lotti,[b] Francesco Pagliaro,[b] Marco Merlini[b]

[a]*Dipartimento di Scienze della Terra, dell'Ambiente e della Vita (DISTAV), Università degli Studi di Genova, Italy. donato.belmonte@unige.it*
[b]*Dipartimento di Scienze della Terra 'A. Desio', Università degli Studi di Milano, Milano, Italy*

Although grossite ($CaAl_4O_7$) is an important constituent phase of high alumina cements (HAC) and a common refractory phase in calcium-rich inclusions (CAIs) found in primitive chondritic meteorites, its thermophysical properties are poorly constrained and its thermodynamic behaviour mostly unknown. In particular, the knowledge of phase stability relations up to high pressure and temperature conditions (HP-HT) is concealed by the lack of informations on elasticity and P-V-T equation of state parameters.
Thermodynamics, equation of state and elasticity of grossite (space group *C*2/c) have been investigated in this work by first principles theory (using a WC1LYP hybrid functional and CRYSTAL program) and experimental methods (synchrotron radiation high-pressure single crystal X-ray diffraction, using an ETH-type Diamond Anvil Cell and M.E.W. as pressure-transmitting fluid, at Xpress beamline at Elettra, Trieste, λ = 0.4957 Å) in a broad range of P-T conditions (i.e. 0-10 GPa and 0-2000 K).
HP experiments reveal a displacive first order phase transition, which has been observed between 6.1 and 7 GPa by ca. a 3% change in lattice volume and the violation of *C*-centring extinction conditions. In fact, the symmetry changes by losing the centring of the lattice and the centre of symmetry, passing from *C*2/*c* to *Pc* space group. The phase transition is marked by a dramatic change of the isothermal bulk modulus (K_o) from 123(4) GPa in the low-pressure regime to 35(8) GPa in the high-*P* phase, which shows a very soft and anisotropic behaviour. First principles calculations provide static EoS parameters [e.g. K_0 = 128.8(1) GPa and K'_0 = 4.0(1) for the *C*2/*c* phase], which are in remarkable agreement with experiments. Furthermore, ab initio calculation of the full elastic tensor (with 13 independent components) permits to define the shear modulus (i.e. G_{VRH} = 52.1 GPa) and seismic anisotropy of the C2/c phase, for which no experimental data exist so far. Seismic anisotropy of P-, S1- and S2-waves turns out to be equal to A_P=16.0%, A_{S1}=24.7% and A_{S2}=36.3%. A_P and A_{S1} both decrease with pressure, while A_{S2} increase up to a huge value (ca. 58.8%) at 9 GPa.
Thermodynamic properties have been computed in the framework of quasi-harmonic approximation (QHA) by phonon dispersion calculations on 2×2×2 supercells to reach numerical convergence. The calculated heat capacity and standard-state entropy values shows a good agreement with the available calorimetric data. P-V-T relations have been obtained by a first-principles Mie-Gruneisen EoS [1] and permitted to calculate Gibbs free energy in the invetigated P-T range. Due to high computational cost, thermodynamic properties of the P*c* phase have been defined by a modified Kieffer's model approach splitting acoustic and optic contributions and defining the former from the ab initio elastic constant tensor, the latter from vibrational frequencies calculated at Γ-point [2]. A temptative phase transition boundary for the *C*2/*c* → P*c* reaction is thus predicted by Gibbs free energy minimization. Finally, ab initio thermodynamic properties of grossite have been used to constrain its phase stability field in the CaO-Al_2O_3-SiO_2 (CAS) ternary system at HP-HT along the guidelines defined in a previous study [3].

[1] D. Belmonte *Minerals*. **2017**, *7*, 183.
[2] D. Belmonte, C. Gatti, G. Ottonello, P. Richet *J. Phys. Chem. A.* **2016**, *120*, 8881.
[3] G. Ottonello, M. Attene, D. Ameglio, D. Belmonte, M. Vetuschi Zuccolini, M. Natali *Chem. Geol.* **2013**, *346*, 81.