RESIDUAL STRESS MEASUREMENT OF YB SILICATES BY RAMAN SPECTROSCOPY: FIRST-PRINCIPLES AND EXPERIMENTAL STUDIES

Takafumi Ogawa, Japan Fine Ceramics Center
t_ogawa@jfcc.or.jp
Yoshihisa Tanaka, National Institute of Materials Science
Taishi Yokoi, Japan Fine Ceramics Center
Hideki Kakisawa, National Institute of Materials Science
Satoshi Kitaoka, Japan Fine Ceramics Center

Key Words: Environmental barrier coating, Yb silicates, Residual stress, Raman microscopy, First-principles simulation

Components of next-generation gas turbines made from lightweight SiC-based ceramics need environmental barrier coatings (EBCs) to protect from water vapor at high temperature because Si-based ceramics vaporize in such environments. Yb silicates Yb_2SiO_5 and $Yb_2Si_2O_7$ are promising EBC materials. In EBCs, residual stresses develop during thermal cycling due to mismatch between the thermal expansion coefficients of the silicate and the underlying ceramics, resulting in critical fatigue of the coating structure [1]. Raman microscopy is one method for measuring stress distributions in coating materials and has the potential to be used for diagnosing EBCs. Its suitability for analyzing stress states of Yb silicates has been unknown.

In this study, we examine Raman spectra of Yb_2SiO_5, and $Yb_2Si_2O_7$ under hydrostatic pressure based on first-principles calculations based on the density functional theory and we also examine the spectra of $Yb_2Si_2O_7$ under uniaxial compressive stress in experiments using polycrystalline samples. When no external pressures applied, good agreement between calculated and experimental spectra is obtained as shown in Figure 1. The differences in the spectra between the silicates demonstrate the utility of using Raman microscopy to detect compositional changes in Yb-silicate coatings. From the calculations, lattice vibrations associated with a Raman peak are identified as exemplified by the characteristic mode of Si_2O_7 units in $Yb_2Si_2O_7$ shown in figure 1(a).

The calculated changes in Raman spectra as a function of pressure are as large as those for yttria-stabilized zirconia, suggesting that Raman microscopy is suitable for monitoring residual stresses in both Yb silicates. This is experimentally confirmed for the large intensity peaks at around 950 cm^{-1} of $Yb_2Si_2O_7$.

This work was partially supported by the Cross-ministerial Strategic Innovation Promotion Program (SIP) “Structural Materials for Innovation” (Japan Science and Technology Agency).

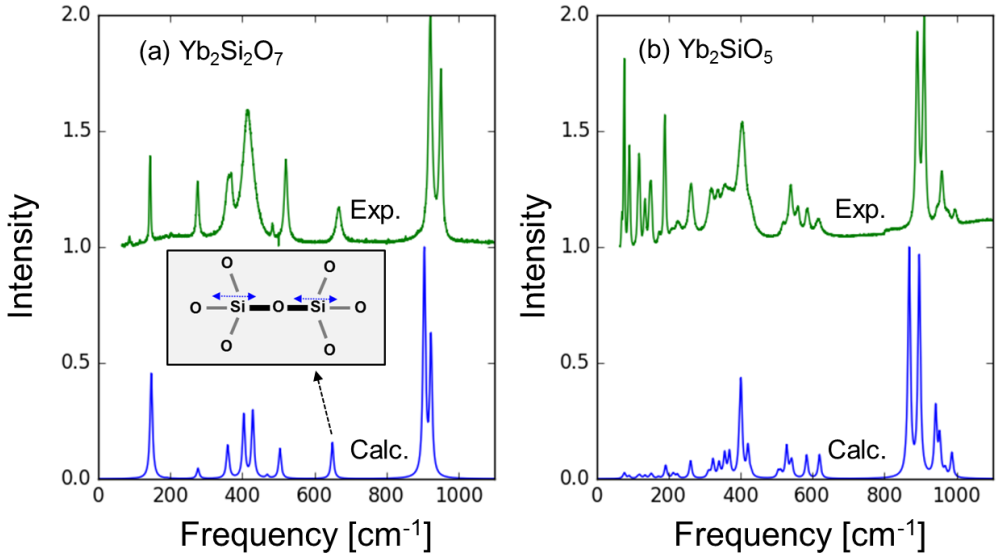

Figure 1 Measured and calculated Raman spectra of (a) $Yb_2Si_2O_7$ and (b) Yb_2SiO_5 with no external pressure.

[1] A. G. Evans et al., Prog. Mater. Sci. 46, 505 (2001).