Institut de Minéralogie et de Physique des Milieux Condensés
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SÉMINAIRE
Lundi 14 novembre, 10h30

Salle de Conférence, 4ème étage, Tour 22-23, Salle 1
IMPMC, Université P. et M. Curie, 4, Place Jussieu, 75005 Paris

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GIANT NEGATIVE THERMAL EXPANSION DRIVEN BY INTERMETALLIC CHARGE TRANSFER IN $BiNiO_3$

The unusual property of negative thermal expansion (NTE) is of fundamental interest and may be used to fabricate composites with controlled thermal expansion values. Systems, such as ZrW_2O_8, show NTE over a wide temperature range. NTE can result from transitions between different electronic or magnetic states coupled to the lattice, as in the case of $(Mn_{0.96}Fe_{0.04})_3(Zn_{0.5}Ge_{0.5})N$. $BiNiO_3$ is an antiferromagnetic insulator with a unique charge distribution of $Bi^{3+}_{0.5}Bi^{5+}_{0.5}Ni^{2+}O_3$. It shows a 2.6% volume reduction under pressure due to a Bi/Ni charge transfer accompanied by an insulator to metal transition. The charge transfer transition is shifted to ambient pressure through La substitution for Bi. We found that the relative proportion of the low- and high-T phases changes as a function of temperature, thus leading to a smooth volume decrease upon heating. By means of dilatometric measurements, the linear expansion coefficient of a $Bi_{0.95}La_{0.05}NiO_3$ pellet was measured to be $-137\times10^{-6}K^{-1}$ at RT and $-82\times10^{-6}K^{-1}$ in the 320-380 K range.

[1] S. Ishiwata *et al.*, J. Mater. Chem. 12, 3733 (2002).
[2] M. Azuma *et al.*, J. Am. Chem. Soc. 129, 14433 (2007).
[3] S. Ishiwata *et al.*, Phys. Rev. B 72, 045104 (2005).
[4] M. Azuma *et al.*, Nature Commun. 2, 347 (2011).

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