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Can oxygen deficient SmFeAsO$_{1-x}$ be synthesized?: Unintentional incorporation of hydride ion at oxygen vacancy site

YOSHINORI MURABA, Materials Research Center for Element Strategy, SOSHI IIMURA, Materials and Structures Laboratory, Tokyo Institute of Technology, SATORU MATSUISHI, HIDEO HOSONO, Materials Research Center for Element Strategy, Tokyo Institute of Technology —

Hydrogen substitution and introduction of oxygen vacancy are effective electron doping methods for the *Ln*FeAsO. However, their T_c vs e$^-$/Fe diagrams do not entirely overlap each other, while T_c vs lattice dimension relationships are very similar. These contradictions can be understood by assuming that unintentional hydrogen is incorporated into the oxygen vacancy. To examine the preferred electron-dopant species in *Ln*FeAsO and the influence of the atmosphere during synthesis on the formation of *Ln*FeAsO$_{1-x}$, we try to synthesize the SmFeAsO$_{1-x}$ under three well-controlled atmosphere (H_2O, H_2 and H_2O- and H_2-free). Under H_2O and H_2 atmosphere, hydrogen were incorporated at oxygen sites as the hydride ion and SmFeAsO$_{1-x}$H$_x$ was formed. On the other hand, when H_2O and H_2 were removed from synthetic process, nearly stoichiometric SmFeAsO was formed. Furthermore, DFT calculations showed that H-substituted samples are more stable than oxygen deficient samples. These results strongly imply that the reported *Ln*FeAsO$_{1-x}$ was contaminated with unintentional hydrogen and *Ln*FeAsO$_{1-x}$H$_x$ was misidentified as *Ln*FeAsO$_{1-x}$.

Yoshinori Muraba
Materials Research Center for Element Strategy

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