Synthesis, Characterization and Chemical Stability of Silicon Dichalcogenides, $Si(Se_xS_{1-x})_2$

Chen Chen, Xiaotian Zhang, Lakshmi Krishna, Chito Kendrick, Shun-Li Shang, Eric Tobereb, Zi-Kui Liu, Adele Tamboli, Joan M. Redwing

www.elsevier.com/locate/jcrysgro

PII: S0022-0248(15)00715-0
DOI: http://dx.doi.org/10.1016/j.jcrysgro.2015.12.005
Reference: CRYS23096

To appear in: *Journal of Crystal Growth*

Received date: 30 September 2015
Revised date: 23 November 2015
Accepted date: 4 December 2015

Cite this article as: Chen Chen, Xiaotian Zhang, Lakshmi Krishna, Chit Kendrick, Shun-Li Shang, Eric Tobereb, Zi-Kui Liu, Adele Tamboli and Joan M. Redwing, Synthesis, Characterization and Chemical Stability of Silico Dichalcogenides, $Si(Se_xS_{1-x})_2$, *Journal of Crystal Growth* http://dx.doi.org/10.1016/j.jcrysgro.2015.12.005

Synthesis, Characterization and Chemical Stability of Silicon Dichalcogenides, $Si(Se_xS_{1-x})_2$

Chen Chen[1], Xiaotian Zhang[1], Lakshmi Krishna[2], Chito Kendrick[3], Shun-Li Shang[1], Eric Toberer[2, 4], Zi-Kui Liu[1], Adele Tamboli [4], and Joan M. Redwing[1]*

[1]Department of Materials Science and Engineering, Materials Research Institute, Pennsylvania State University, University Park, PA 16802, United States.

[2]Department of Physics, Colorado School of Mines, CO 80401, United States.

[3]Department of Electrical and Computer Engineering, Michigan Technological University, MI 49931, United States.

[4]National Center for Photovoltaics, National Renewable Energy Laboratory, Golden, CO 80404, United States.

ABSTRACT

Silicon dichalcogenides have an intriguing crystal structure consisting of long tetrahedral chains held together by van der Waals forces but the electronic and optical properties have been less explored. In the present work, bulk $SiSe_2$, SiS_2, and $Si(Se_xS_{1-x})_2$ were synthesized by the congruent melt growth method and characterized by Raman spectroscopy, X-ray Diffraction and UV/visible/IR transmission measurements supported by first-principles calculations. First-principles calculations reveal a nearly linear decrease of band gap energy in $Si(Se_xS_{1-x})_2$ with increasing Se content, i.e., from SiS_2 to $SiSe_2$ which corresponds with a blue-shift in the transmission spectra from bulk $SiSe_2$ to $Si(Se_{0.6}S_{0.4})_2$, and to SiS_2. Air stability tests demonstrate the formation of toxic H_2Se/H_2S gas from sample oxidation at room temperature upon exposure to ambient air, and great care should be paid when handling these materials.

KEYWORDS

A1. Characterization, A1, Computer simulation, A2. Growth from melt, B1. Sulfides, B3. Solar cells,