

カルコゲン合金の物性

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2000 Fiscal Year Final Research Report Summary

Properties of chalcogen alloys

Research Project

Project/Area Number

11640343

Research Category

Grant-in-Aid for Scientific Research (C)

Allocation Type

Single-year Grants

Section

一般

Research Field

固体物性Ⅱ(磁性・金属・低温)

Research Institution

Kanazawa University

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Research Abstract

(1) First-principles electronic structure calculations have been carried for all high-pressured phases (Se-I, II, III, IV, X, VI) of Selenium with using a full-potential augmented plane wave (FLAPW) method, based on the density functional theory (LDA and GGA calculation), and the pressure-induced phase transitions have been discussed. Through the transition, Se-I→Se-II, the trigonal chain in Se-I is folded on a plane. Lone-pair orbitals which exist on all atoms in Se-I vanish partially in Se-II and entirely in Se-III. The electronic structure in Se-III shows a complete metallic behavior. A new structure of Se-IV have been proposed, which could reasonably explain a second-order property of the phase transition between Se-IV and V. The proposed structure is consistent with the extinction law of the X-ray diffraction measurement and the space group of Se-IV have been determined to be $P2_1/m$. The transition pressure between Se-V and VI has been estimated from the total energy calculation and ... More

Research Products (24 results)

All Other

All Publications (24 results)

- [Publications] Y.Kawakita, M.Yao and H.Endo: "Short and long bonds in liquid tellurium" *J.Non-cryst.Solids.* 250-252. 447-452 (1999) ▼
- [Publications] H.Endo, H.Hoshino, H.Ikemoto and T.Miyanaga: "Semiconductor-metal transition in liquid As-Te mixtures" *J.Phys.: Condensed Matter.* 12. 6077-6099 (2000) ▼
- [Publications] H.Hoshino, I.Yamamoto, T.Miyanaga, H.Ikemoto and H.Endo: "The electronic and structural changes in the supercooled liquid and glassy As₂Se₃" *J.Non-cryst.Solids.* 250-252. 478-482 (1999) ▼
- [Publications] T.Miyanaga, H.Hoshino, H.Ikemoto, I.Yamamoto, H.Endo: "EXAFS studies of liquid chalcogenides" *Jpn.J.Appl.Phys.* 38. 560-563 (1999) ▼
- [Publications] H.Ikemoto, H.Hoshino, T.Miyanaga, I.Yamamoto and H.Endo: "The semiconductor-metal transition of liquid tellurium-arsenic mixtures" *J.Non-cryst.Solids.* 250-252. 458-462 (1999) ▼
- [Publications] K.Nakamura and A.Ikawa: "Inter-chain interaction in semi-conducting liquid and amorphous selenium" *Prog.Theor.Phys.Supp.* 138. 266-267 (2000) ▼
- [Publications] K.Nakamura and A.Ikawa: "Infrared absorption in amorphous selenium" *Compt.Phys.Commun.*, (印刷中). ▼
- [Publications] F.Shimizu, H.Kaburagi, T.Oda and Y.Hiwatari: ""Chain Structure of Liquid and Amorphous Selenium : Tight-Binding Molecular-Dynamics Simulation"" *J.Non-Cryst.Solids.* 250-252. 433-436 (1999) ▼
- [Publications] M.Geshi, T.Oda and Y.Hiwatari: ""The Electronic Structure of a High Pressure Monoclinic Selenium and the Structural Phase Transition"" *J.Phys.Soc.Jpn.* 68. 3341-3346 (1999) ▼
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- [Publications] M.Geshi, T.Oda and Y.Hiwatari: ""Electronic Structure and Structural Stability of the High-Pressured Orthorhombic Phase of Selenium"" *J.Phys.: Condens.Matter.* (印刷中). ▼
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