

# Properties of chalcogen alloys

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# 2000 Fiscal Year Final Research Report Summary

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## Properties of chalcogen alloys

Research Project

### Project/Area Number

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11640343

### Research Category

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Grant-in-Aid for Scientific Research (C)

### Allocation Type

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Single-year Grants

### Section

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一般

### Research Field

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固体物性Ⅱ(磁性・金属・低温)

### Research Institution

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Kanazawa University

### Principal Investigator

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**HIWATARI Yasuaki** Kanazawa University Faculty of Science Professor, 理学部, 教授 (20019491)

### Co-Investigator(Kenkyū-buntansha)

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IKAWA Atsushi Kyoto University Graduate School of Science Assistant Professor, 大学院・理学研究科, 助教授 (80243004)

HOSHINO Hideoki Hirosaki University Faculty of Education Professor, 教育学部, 教授 (30001861)

ENDO Hirohisa Fukui Institute of Technology Faculty of Engineering Professor, 工学部, 教授 (40025284)

HIROYUKI Ikemoto Toyama University Faculty of Science Assistant, 理学部, 助手 (20262496)

TATUKI Oda Kanazawa University Faculty of Science Lecturer, 理学部, 講師 (30272941)

### Project Period (FY)

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1999 – 2000

### Keywords

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metal-insulator transition / liquid-liquid transition / chalcogenes / infrared absorption / tight binding molecular dynamics / polarization / 高圧セレン / FLAPW / 電子状態

## 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.Miyayaga: "Semiconductor-metal transition in liquid As-Te mixtures" J.Phys.: Condensed Matter. 12. 6077-6099 (2000)		▼
[Publications] H.Hoshino, I.Yamamoto, T.Miyayaga, H.Ikemoto and H.Endo: "The electronic and structural changes in the supercooled liquid and glassy As <sub>2</sub> Se <sub>3</sub> " J.Non-cryst.Solids. 250-252. 478-482 (1999)		▼
[Publications] T.Miyayaga, 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.Miyayaga, 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).		▼
[Publications] M.Geshi, T.Oda and Y.Hiwatari: ""Electronic Structures and Phase Transitions of Selenium under High Pressure"" Active Report 1999 Supercomputer Center MDCL ISSP University of Tokyo. 67-68 (1999)		▼
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[Publications] H.Endo, H.Hoshino, H.Ikemoto and T.Miyayaga: "Semiconductor-metal transition in liquid As-Te mixtures" J.Phys.: Condensed Matter. 12. 6077-6099 (2000)		▼
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