obtained by X-ray diffraction and Raman spectroscopy. The chemical stoichiometry was determined by X-ray photoelectron spectroscopy (XPS), obtaining WO_3. By X-ray diffraction obtained that the as-grown WO_3 films present mainly the crystalline phase monoclinic, whose lattice parameters values: a= 3.8465 Å, b= 7.5449 Å, c= 7.3066 Å, β= 90.924°. The Raman spectrum of the as-deposited film shows intense peaks at 801, 710, 262 and 61 cm^{-1}, which are typical Raman peaks of crystalline WO_3 (m-phase) that correspond to the stretching vibrations of the bridging oxygen, which are assigned to W-O stretching (ν) and W-O bending (δ) modes respectively. Annealing WO_3 thin films at the temperatures range from 100 to 500ºC during 10 min in a nitrogen atmosphere; they changed of crystalline phase about 300ºC of monoclinic to orthorhombic, which was corroborated by X-ray diffraction and Raman spectroscopy

Keywords: vibrational, dispersion, X-ray

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Atomic diffusion in liquid B_2O_3 under pressure from *ab initio* molecular dynamics

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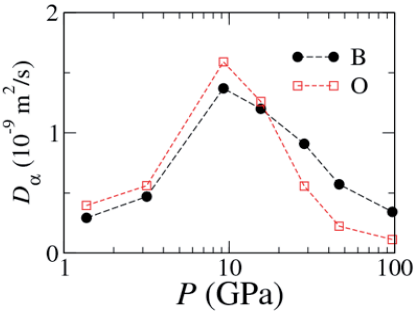
Transport properties of covalent liquids under pressure are very interesting in the sense that they show unexpected pressure dependence. For a number of covalent liquids, such as SiO_2 and GeO_2, the diffusivity of atoms was shown to increase with pressure. It is, however, unclear how the rearrangement process of the covalent bonds is affected by compression.

In order to clarify the microscopic mechanism of atomic diffusion in covalent liquids under pressure, we performed *ab initio* molecular dynamics simulations for liquid B_2O_3 which is a typical covalent liquid.

Figure shows the calculated diffusion coefficients D_α for α=B and O atoms as a function of pressure. Clearly, liquid B_2O_3 has a diffusion maximum around 10 GPa. The decrease in the diffusivity above a certain pressure is not surprising but quite natural. It is, however, unusual that the diffusivity of O atoms is reduced more quickly than that of B atoms with compression above 10 GPa.



We discuss the microscopic origin of this anomalous pressure dependence of the diffusivity. Around 10 GPa, covalent bonds are always exchanged by concerted reaction while the non-bridging oxygens (NBO) are needed for atomic diffusion at ambient perssure. These facts suggest that the atomic diffusion with concerted reaction gives the diffusion maximum. At about 100 GPa, almost all B atoms are overcoordinated to O atoms while only 2/3 O atoms are overcoordinated to B atoms. This asymmetry property gives rise to difference in the pressure dependence of the diffusivity. These dynamic properties under pressure will be commonly observed in other covalent liquids, such as SiO_2.

Keywords: ab initio molecular dynamics, high-pressure physics, covalent liquids

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Is there a phase transition between the two liquid states in tin tetraiodide?

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We have reported that in tin tetraiodide there are two liquid states, which are two thermodynamically stable counterparts of the metastable amorphous solid states [1]. This finding was established by in-situ synchrotron x-ray diffraction measurements, which were carried out under high pressures up to about 4 GPa.

However, no clear-cut experimental evidence has been obtained as to the existence of phase transition between the two liquid states, although the mean-field theoretical analyses of the experimental findings based on both Son-Patashinski's [2] and Franzese-Stanley's [3] models support the existence of a first-order transition [4].

In order to clarify the point, a close examination was made around the region in question in the temperature-pressure phase diagram. This includes in-situ measurements of structure and density using synchrotron x-ray diffraction and absorption. Variation of the local structure, which is characterized by a suitably defined local order parameter, showed a smooth behavior with pressure, implying a gradual change in the *local* structure. However, a jump, though very subtle, in the density variation on compression was detected at around 970 K and 1.5 GPa, just above the break point in the melting curve of the low-pressure crystalline state. The result is to be reconfirmed in the near future.

We have also examined on the theoretical side the Son-Patashinski model in some detail. To go beyond the mean-field calculations, the effects of fluctuations on the stability of the phases were investigated using a lattice version of the model. The transition between the two liquid phases was, unlike mean-field's prediction, found to be smeared out partially by the finite size effects of the system. To extract the exact nature of the transition, which the model possesses, the multicanonical ensemble simulations are currently in progress.

In conclusion, there is a phase transition between the two liquid states in tin tetraiodide, but the transition is of weak first order.

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Keywords: phase, liquid, pressure

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Structure of liquid transition metal hydrogen alloys under high pressure

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Hydrogen reacts with many metals and form metal hydrides. In transition metal hydrides, hydrogen atoms usually occupy interstitial sites and the crystalline lattice expands. Though there are many studies on crystalline metal hydrides, almost nothing is known about liquid