Structural and Vibrational Study of Pseudocubic $CdIn_2Se_4$ under Compression

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Supplementary material

During one of the RS experiments, we noted that when the laser power is high enough (P > 10 mW), the sample near 7 GPa absorbs the laser radiation and heats thus leading to a change in the RS spectrum. To analyze the heating effect we decrease pressure down to 0.7 GPa and we measured the burned sample during a second pressure upstroke as shown in **Figure S1a** in the supplementary material. The pressure dependence of the four Raman-active modes observed in the burned sample are shown in **Figure S1b** in the supplementary material. A close comparison with similar measurements performed in $HgGa_2Se_4$[1] and in other chalcogenides containing Se and Te[2] under similar excitation conditions show that all four peaks observed in $CdIn_2Se_4$ correspond to trigonal Se[3,4]. Therefore, we conclude that PS-$CdIn_2Se_4$ undergoes decomposition at high pressures close to the phase transition pressure under strong laser heating. The decomposition of PS-$CdIn_2Se_4$ into CdSe and In_2Se_3 was previously reported at P > 2 GPa and T > 350 °C [5]. However, our Raman spectra give no hint regarding the possible observation of CdSe[6] or In_2Se_3[7] and only trigonal Se seems to be observed. Therefore, this experiment stresses the importance of controlling laser excitation in order to avoid local heating effects that could cause the decomposition of chalcogenide compounds.

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Figure S1. (Color online) (a) Room temperature Raman scattering spectra of $CdIn_2Se_4$ at selected pressures up to 14.8 GPa in burned zones of the sample. (b) Pressure dependence of the experimental mode frequencies in the burned zones of $CdIn_2Se_4$. The observed Raman peaks and their pressure dependence match perfectly with trigonal Se (see supplementary text).

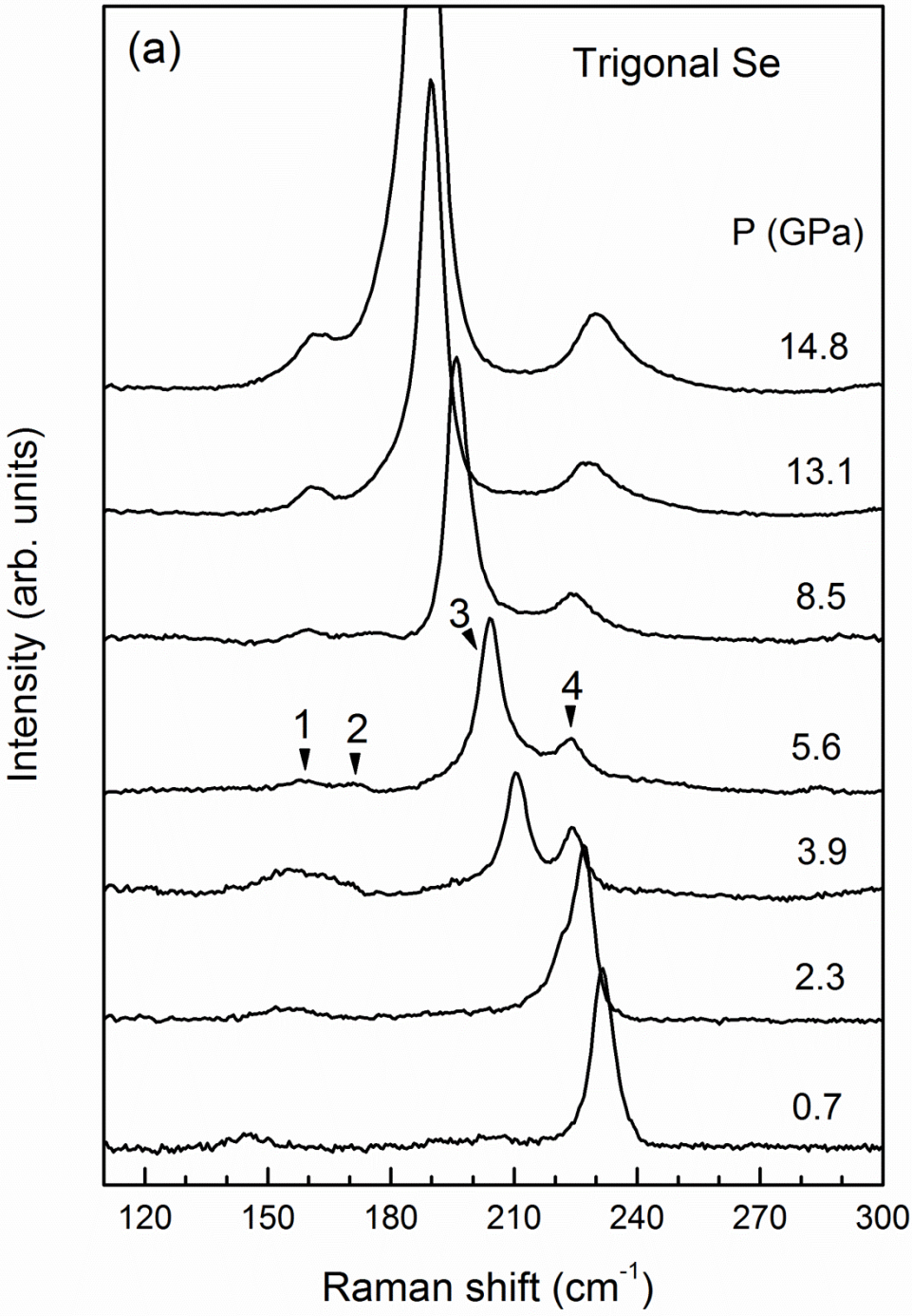
(a)
Trigonal Se
P (GPa)
14.8
13.1
8.5
5.6
3.9
2.3
0.7
1
2
3
4
Intensity (arb. units)
120
150
180
210
240
270
300
Raman shift (cm-1)

Figure S1a

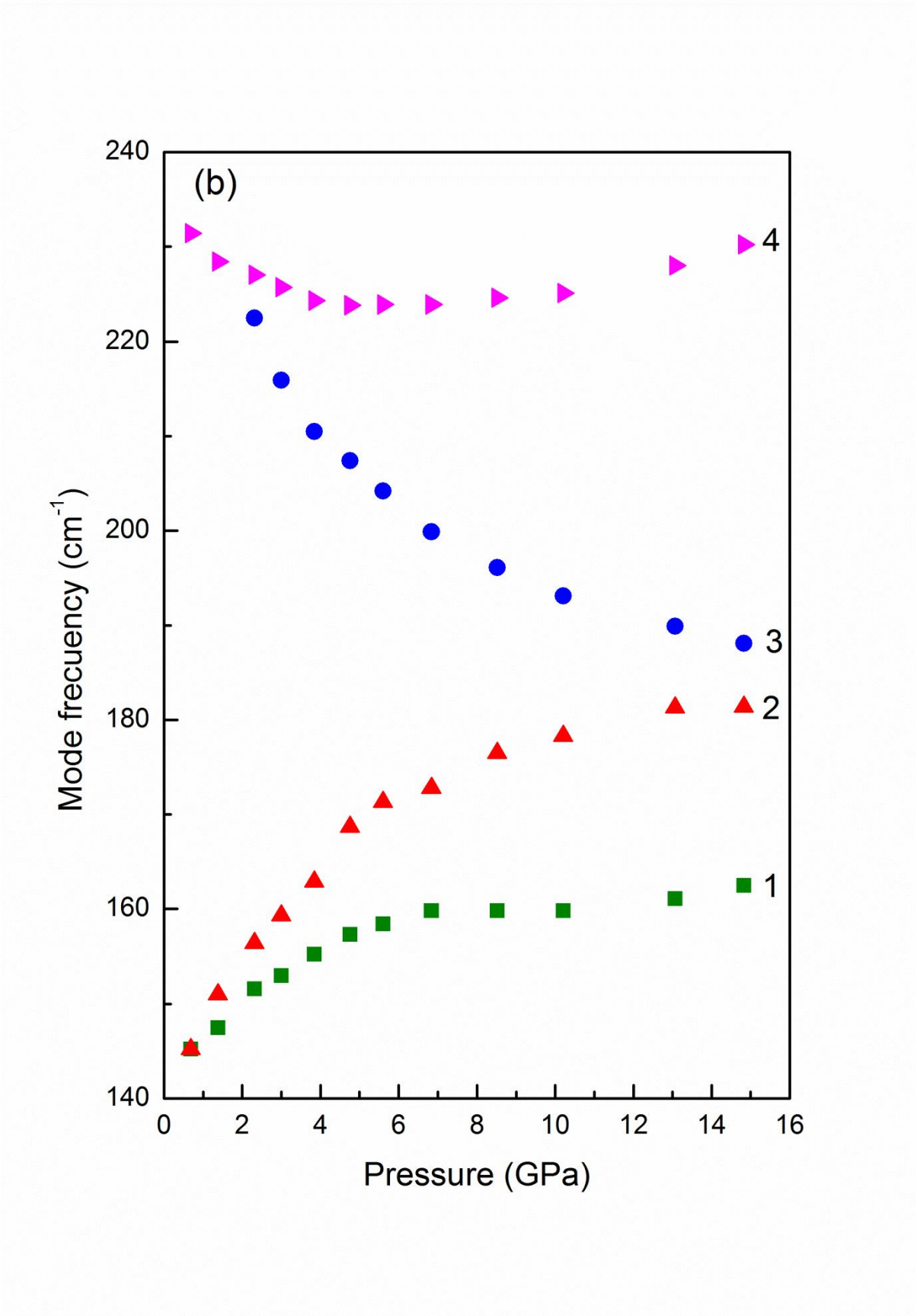
(b)
Mode frecuency (cm-1)
Pressure (GPa)
240
220
200
180
160
140
0
2
4
6
8
10
12
14
16
1
2
3
4

Figure S1b