C2S_0301* is a designation of the samples. All samples are parts of one ingot (C2S_0301).

Results of the measurements performed are designated as follows: (sample ID)-(type of measurement)-(number of measurement of the sample)-(date).

For the data used in a paper "The unstable thermoelectric effect in non-stoichiometric Cu2Se during the non-equilibrium phase transition", a number of the appropriate figure is provided.

Thermoelectric measurements results

The following files contain raw data of the thermoelectric properties measurements. Data columns are described in the headings of the files.

C2S_0301E-LSR-1-200721.ASC and C2S_0301E-LSR-2-200722.ASC are results of stability measurements. Each measurement (file) consists of two thermal cycles. (One thermal cycle means heating and cooling.) Results are presented in Supplementary Figures S1 and S2.

C2S_0301E-LSR-3-200722.ASC consists of 5 thermal cycles with different heating/cooling rates (set values in the order: 1, 4, 3, 5, 2 K/min). The data is presented in Fig. 3 and S4 (red line - 5 K/min set heating/cooling rate).

C2S_0301E-LSR-5-200923.ASC is a measurement not presented in the paper. The cooling step was stopped at the phase transition temperature to check the stability of the investigated effect. Due to the thermal inertia of the system, the temperature was rippling around the set value.

C2S_0301E-LSR-6-200925.ASC consist of two cycles, initial with 5 K/min heating/cooling rate and the following with 0.1 K/min. The initial results are not used in the paper. The 0.1 K/min one is the "quasi-equilibrium" measurement discussed. Results are presented in Fig. 3 and S4 (black line).

C2S_0301E-LSR-7-201016.ASC contains two cycles with a 5 K/min rate with a different temperature gradient. The initial one is not used and the following is presented in Supplementary Figure S4 (brown line).

DSC results

C2S_0301D2-DSC-1-200811.ngb-dd7 is a raw data file of the DSC measurement. The file can be processed in Netzsch Proteus software.

C2S_0301D2-DSC-1-200811.txt contains the background corrected data exported from the raw data file. The temperature programme and data columns are described in the heading For further processing, sensitivity function (μV/mW) of the 10 K/min measurement was used. For other runs, this function was unreliable. The initial cycle (segments 1-4) was not used. The data is presented in Fig. 4.

XRD results

C2S _0301X-XRD-2-200722.brml is a raw file from the diffractometer. C2S _0301X-XRD-2-200722.txt contains exported data in 2θ (deg.) – Intensity format. The diffraction pattern is presented in Fig. 1.

SEM images and EDX elemental analysis

C2S _0301-SEM-1-200721_***.tif are SEM images. The C2S _0301-SEM-1-200721_008.tif file is used in Fig. 2. C2S_0301-SEM-1-200721_EDXSpetrum.asc is an EDX spectrum of the material, with $Cu_{1.96}Se$ calculated composition. Data columns are described in the heading of the file.

C2S_0301E-SEM-12-210406_EDXSpetrum.asc is an EDX spectrum measured after electrical measurements, with $Cu_{1.92}Se$ calculated composition.

XPS results

C2S_0301E-XPS-11-210323_survey.txt is a wide-range survey spectrum. C2S_0301E-XPS-11-210323_Cu2p.txt and similar Se files contain spectra of the given regions. C2S_0301E-XPS-11-210323_CuLVV.txt is a spectrum of Cu LVV Auger electrons. Data columns are described in the heading of the file. Energies are in eV. The selected regions of the spectrum are presented in Fig. S5.