

Supplementary Information

for

Real structure of $\text{Ge}_4\text{Bi}_2\text{Te}_7$ – Refinement on diffuse scattering data with the 3D- Δ PDF method

Philipp Urban, Arkadiy Simonov, Thomas Weber and Oliver Oeckler

Table S1: Dependent concentrations as a function of refined ones (definitions cf. Table 4).

$C(\text{GB}_1/\text{GB}^1)$	$-1/(12C_3+11C_4+10C_5+9C_6+8C_7+7C_8+6C_9+5C_{10}+4C_{11}+3C_{12}+2C_{13}+C_{14}-15)$
$C(\text{GB}_2/\text{GB}^2)$	$(C_3+C_4-1)/(12C_3+11C_4+10C_5+9C_6+8C_7+7C_8+6C_9+5C_{10}+4C_{11}+3C_{12}+2C_{13}+C_{14}-15)$
$C(\text{V})$	$-1/(12C_3+11C_4+10C_5+9C_6+8C_7+7C_8+6C_9+5C_{10}+4C_{11}+3C_{12}+2C_{13}+C_{14}-15)$
$C(\text{GB})$	$1-(2C_3+2C_4-5)/(12C_3+11C_4+10C_5+9C_6+8C_7+7C_8+6C_9+5C_{10}+4C_{11}+3C_{12}+2C_{13}+C_{14}-15)$
$C(\text{Te}_1/\text{Te}^1)$	$-1/(12C_3+11C_4+10C_5+9C_6+8C_7+7C_8+6C_9+5C_{10}+4C_{11}+3C_{12}+2C_{13}+C_{14}-15)$
$C(\text{Te}_2/\text{Te}^2)$	$(C_3-1)/(12C_3+11C_4+10C_5+9C_6+8C_7+7C_8+6C_9+5C_{10}+4C_{11}+3C_{12}+2C_{13}+C_{14}-15)$
$C(\text{Te})$	$1-(2C_3-4)/(12C_3+11C_4+10C_5+9C_6+8C_7+7C_8+6C_9+5C_{10}+4C_{11}+3C_{12}+2C_{13}+C_{14}-15)$

Table S2: Refined parameters of the disorder model.

scale	0.0963
$\Delta z_i(GB_1/GB^1)$	0.03105
$\Delta z_i(Te_1/Te^1)$	0.01947
$\Delta z_i(GB_2/GB^2)$	0.00719
$\Delta z_i(Te_2/Te^2)$	-0.00190
C_4	0.0432
C_5	0.1474
C_6	0.2665
C_7	0.1810
C_8	0.0927
C_9	0.0762
C_{10}	0.0663
C_{11}	0.0454
C_{12}	0.0235
C_{13}	0.0169
C_{14}	0.0198
$c_{GB1}(\text{Ge})$	0.5258
$c_{GB2}(\text{Ge})$	0.8229
C_3	0 (fixed)
C_{15}	dependent, see manuscript Section 3.5

A YELL input file (model.txt) is deposited as a separate ASCII file along with the dataset (experiment.h5), corresponding weights (weight.h5) and a file that denotes reciprocal space points where no data are measured (reciprocal_space_multiplier.h5).