A mathematical model of amorphous structure of GeTe-Sb_2Te_3 based on crystal-like local structure

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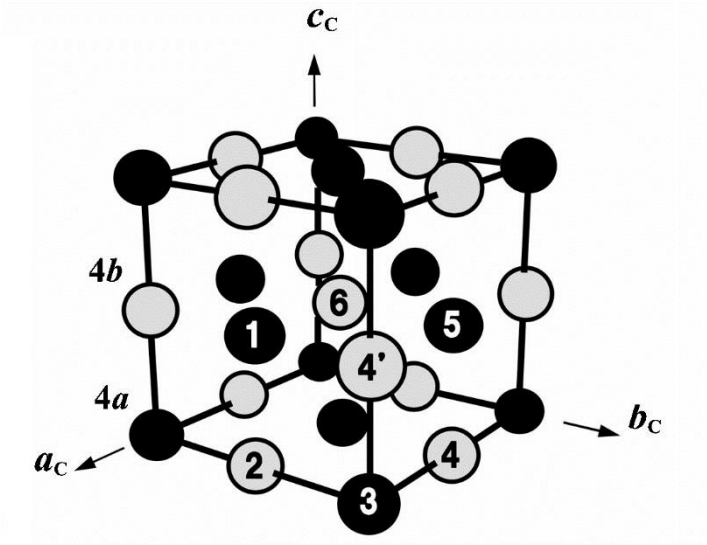
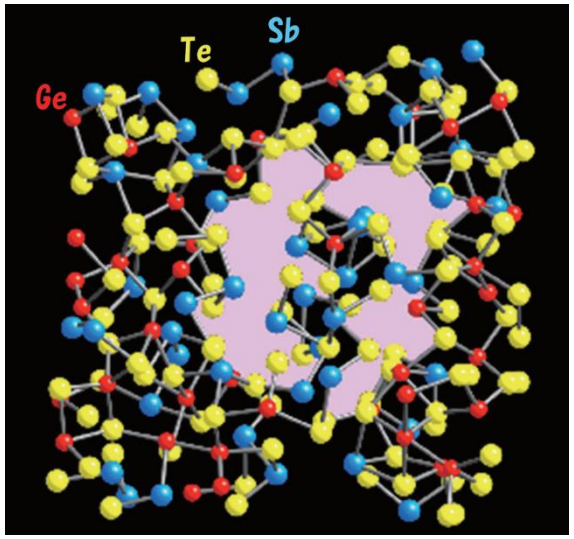
GeTe-Sb_2Te_3

GeTe-Sb_2Te_3 is a phase-change material, which has

Crystal phase (NaCl type) and Amorphous phase





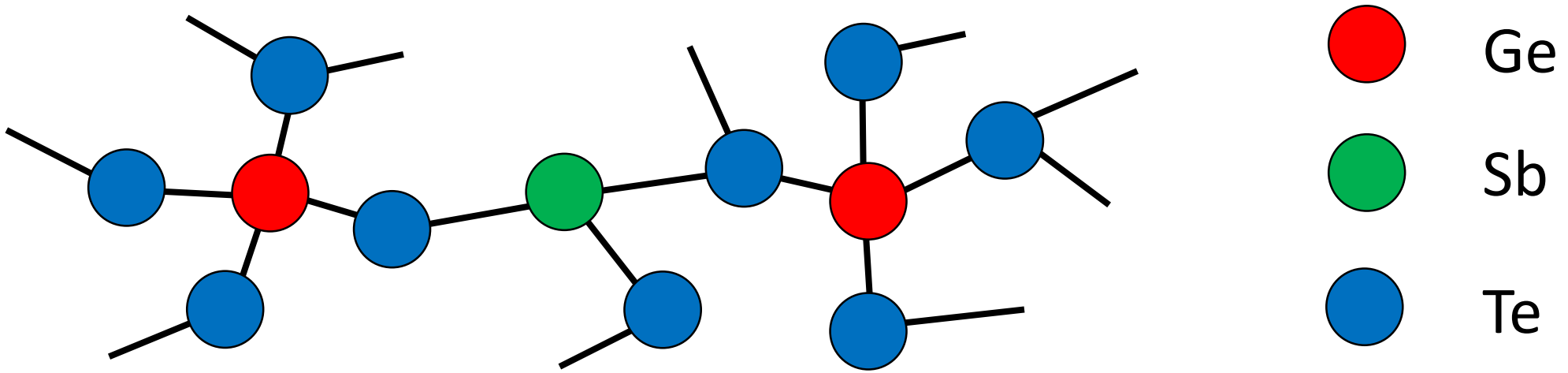
Aim

- Give a simple model of amorphous structure of GeTe-Sb_2Te_3
- Predict a relation between composition ratio and structure

* Pictures are in T. Matsunaga et al., Materia Japan, 89, (2013).

Features of $GeTe$-Sb_2Te_3 in Amorphous phase

- The amorphous structure can be interpreted as the combinations of molecules $GeTe_4$ and $SbTe_3$. *
- The number of covalent bonds of Ge is 4, Sb is 3, Te is 2 or 3. *
- Ge-Te bonds in amorphous phase is especially shorter than them in crystal phase. It's believed that the constitution of Ge-Te covalent bonds is important for the stabilization of the amorphous structure. *



- $GeTe$-Sb_2Te_3 in Amorphous phase may have crystal-like local atomic structure**

* T. Matsunaga et al., Materia Japan, 89, (2013), ** A. Hirata et al, *Nature Mater.* **10**, 28-33 (2011).

Model of Amorphous structure

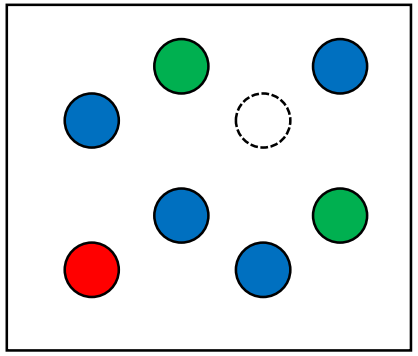
In Crystal phase, Cl-sites are occupied by Te,

Na-site are occupied by Ge, Sb, or Vac (vacancy).

For $(GeTe)_n(Sb_2Te_3)_m$, consider some compositions of 4 Te + 4 (Ge, Sb, or Vac):

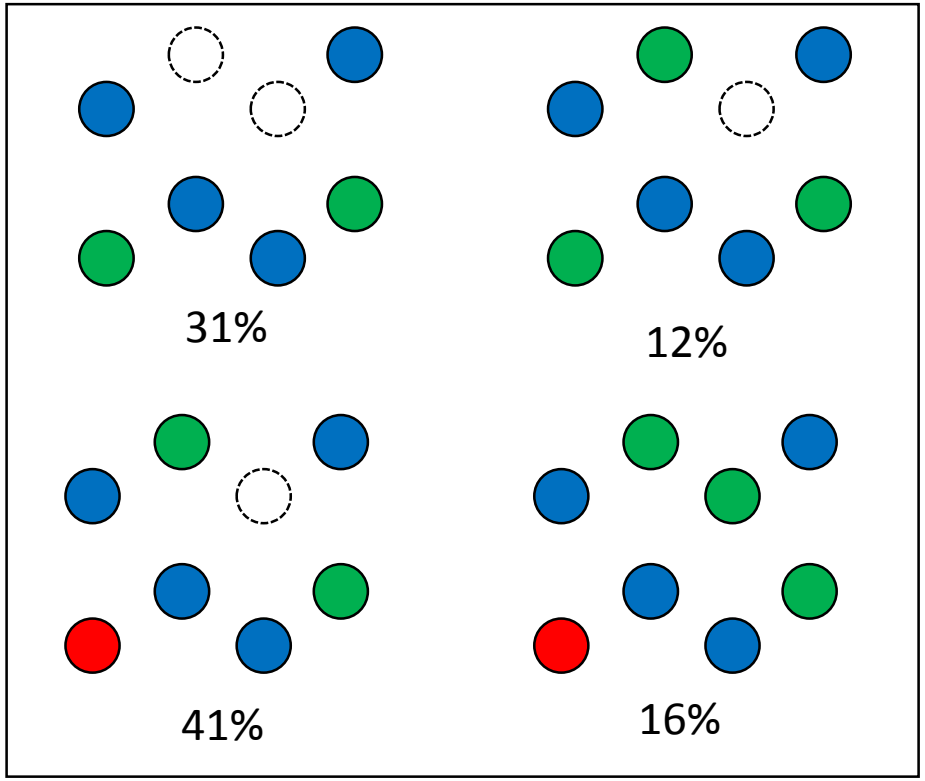
Examples:

$(GeTe)(Sb_2Te_3)$

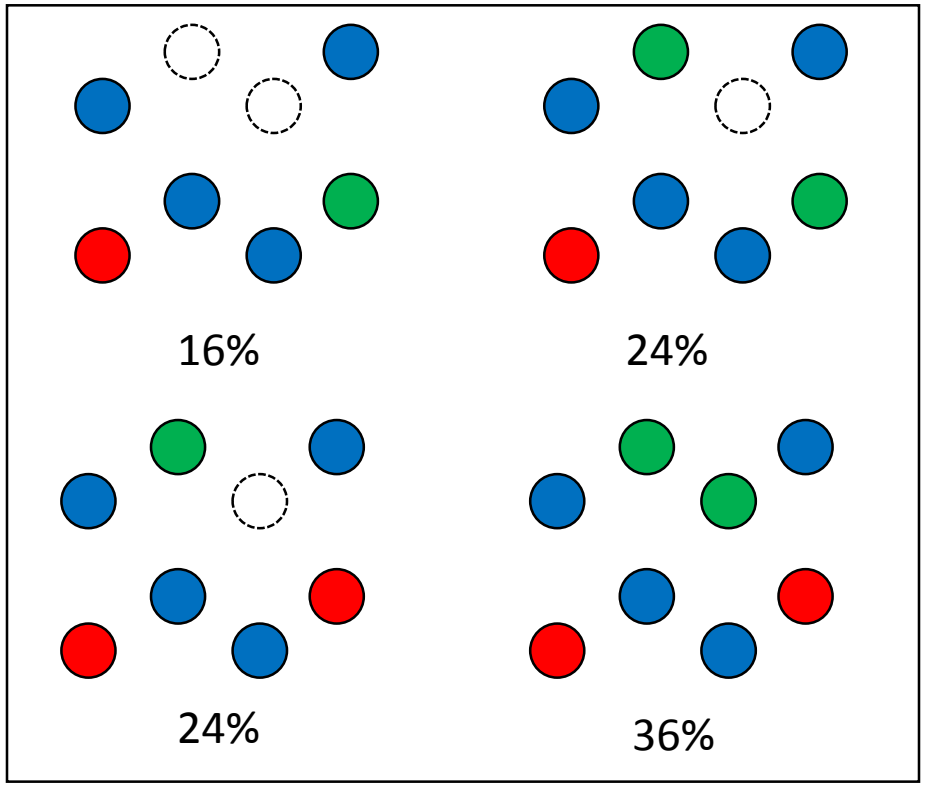


Ge
Sb
Te
Vac

$(GeTe)(Sb_2Te_3)_2$



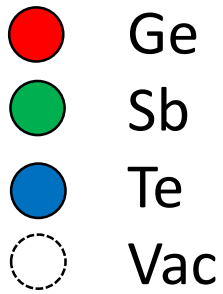
$(GeTe)_2(Sb_2Te_3)$

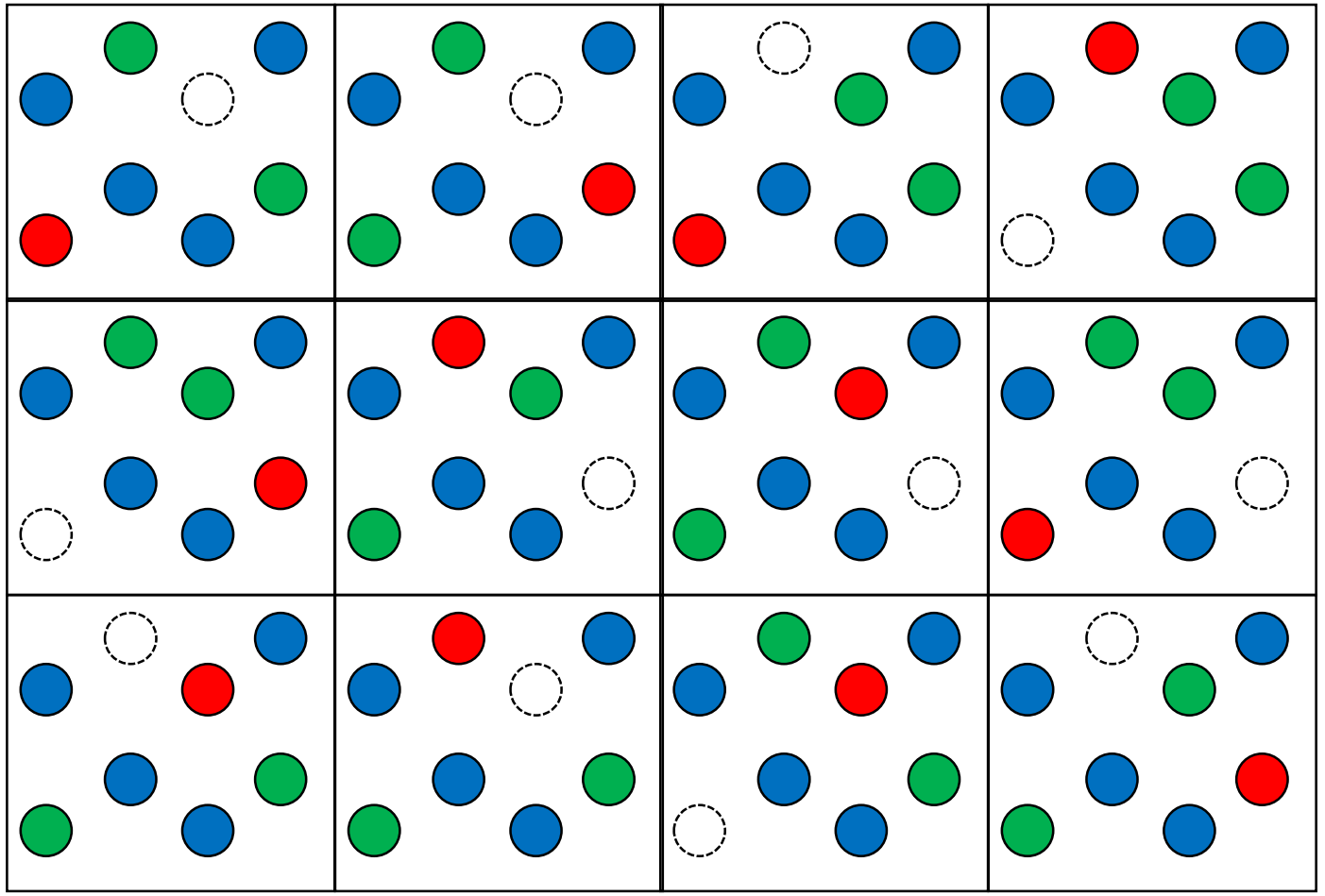


Model of Amorphous structure

(1) Put the compositions of 4 Te + 4 (Ge, Sb, or Vac) on NaCl-crystal sites randomly

Example:
$(GeTe)(Sb_2Te_3)$



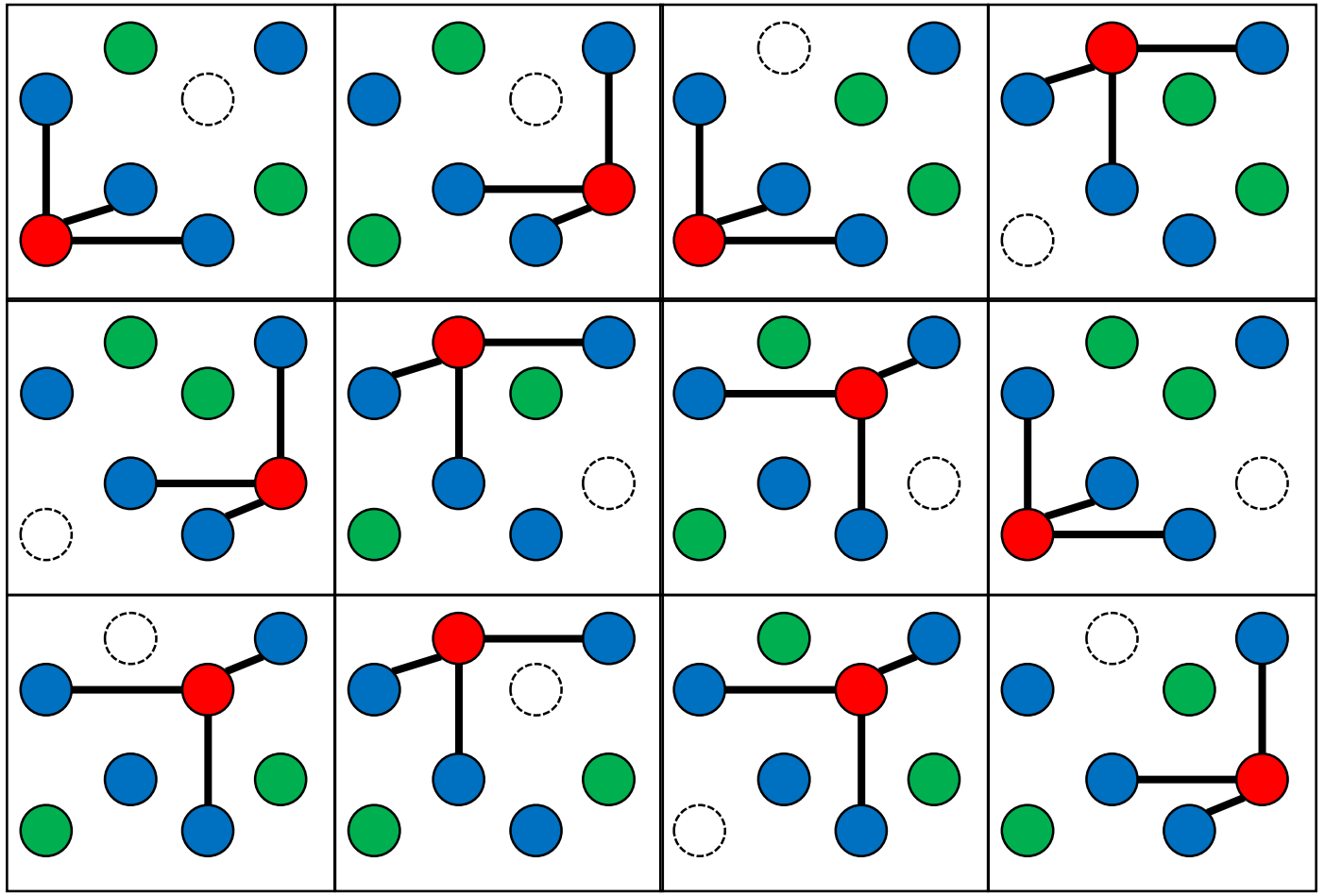


Model of Amorphous structure

(2) Connect each Ge and three Te in the same unit

Example:
$(GeTe)(Sb_2Te_3)$

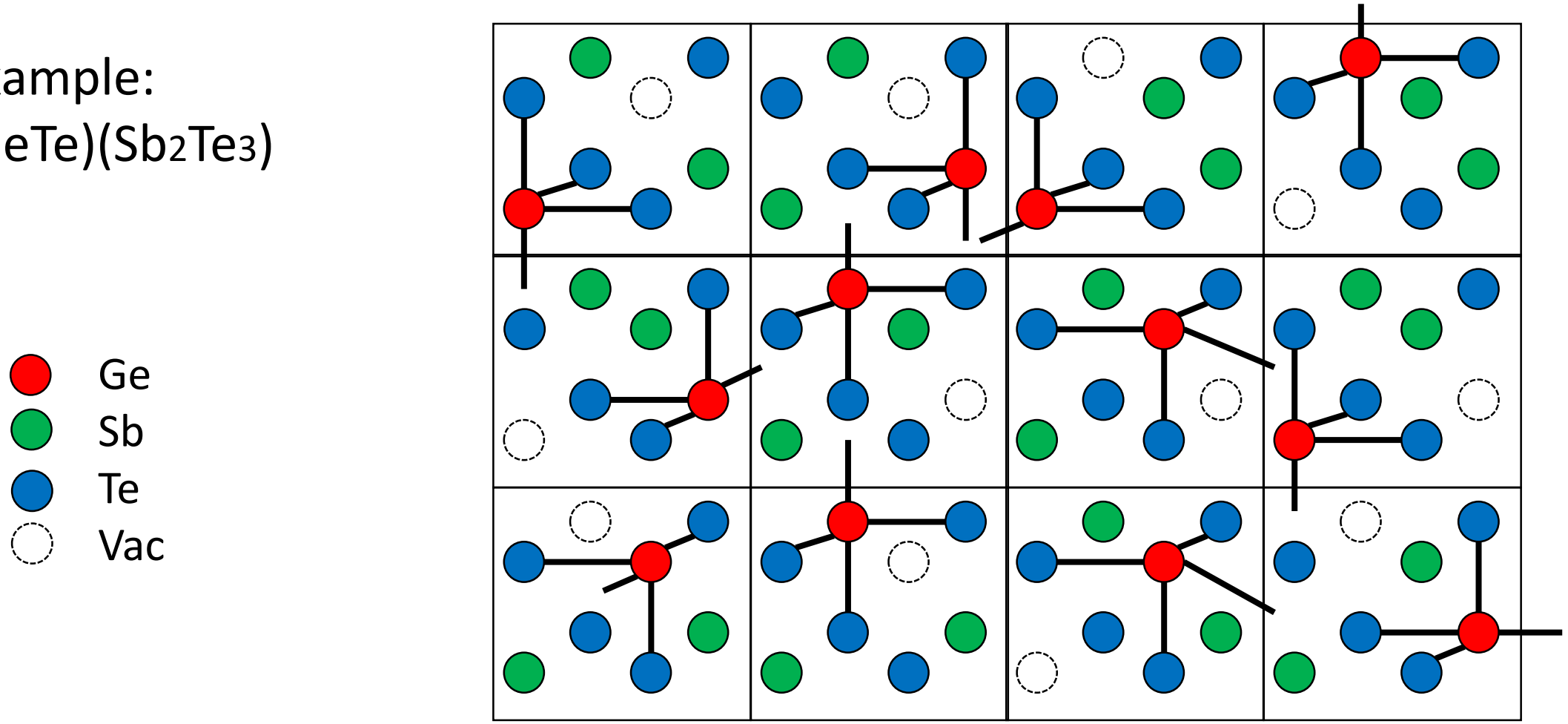
Ge
Sb
Te
Vac



Model of Amorphous structure

(3) For each Ge, choose another unit around it randomly.

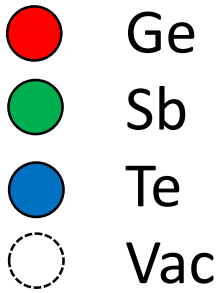
Example:
$(GeTe)(Sb_2Te_3)$

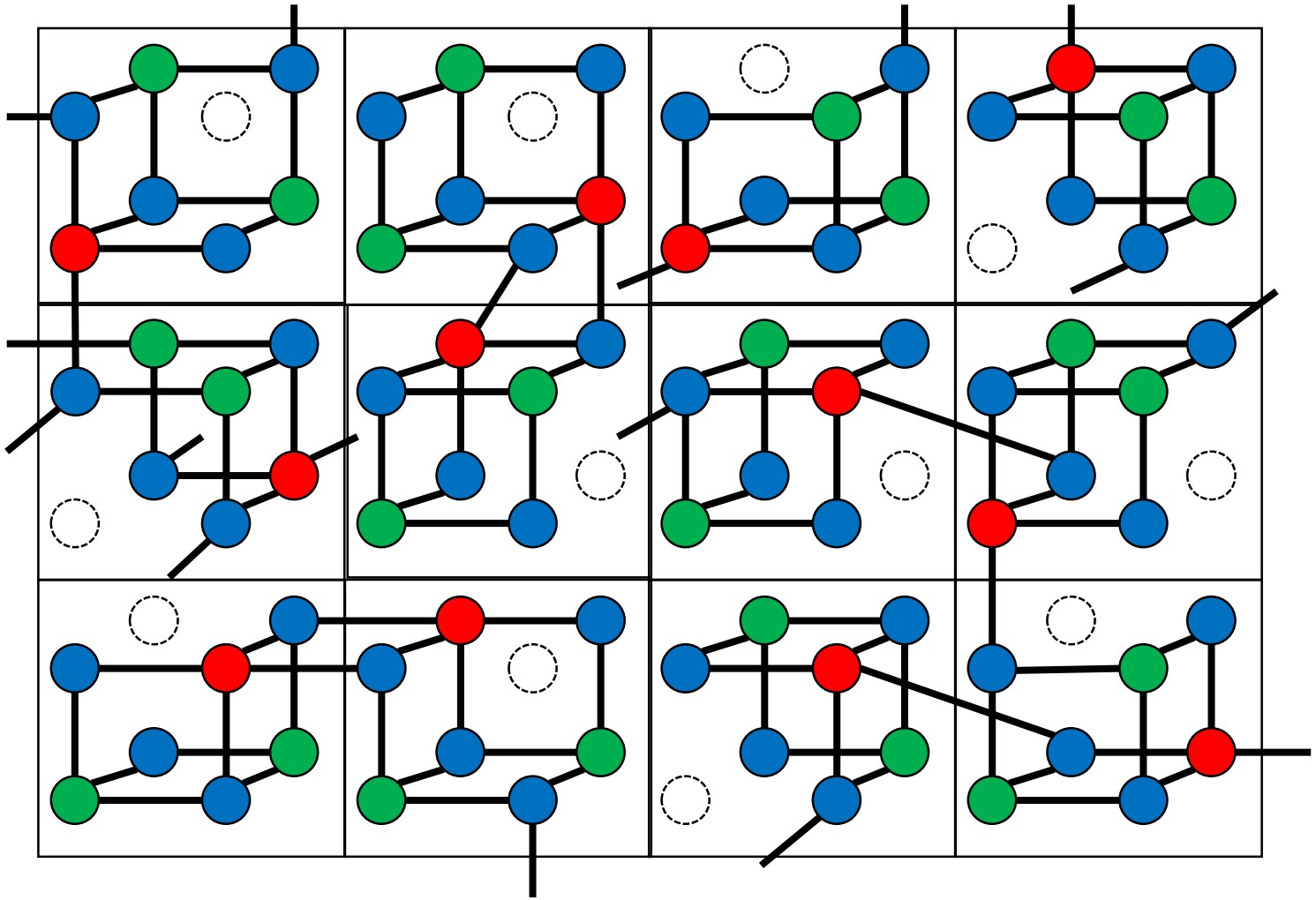


Model of Amorphous structure

(4) Connect Sb and Te in same unit, Ge and Te, Ge and Sb in different units, such that the number of covalent bonds of Ge is 4, Sb is 3, Te is 2 or 3.

Example:
$(GeTe)(Sb_2Te_3)$

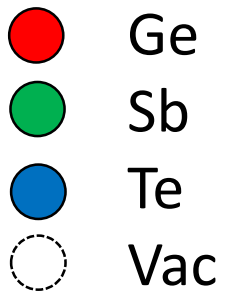


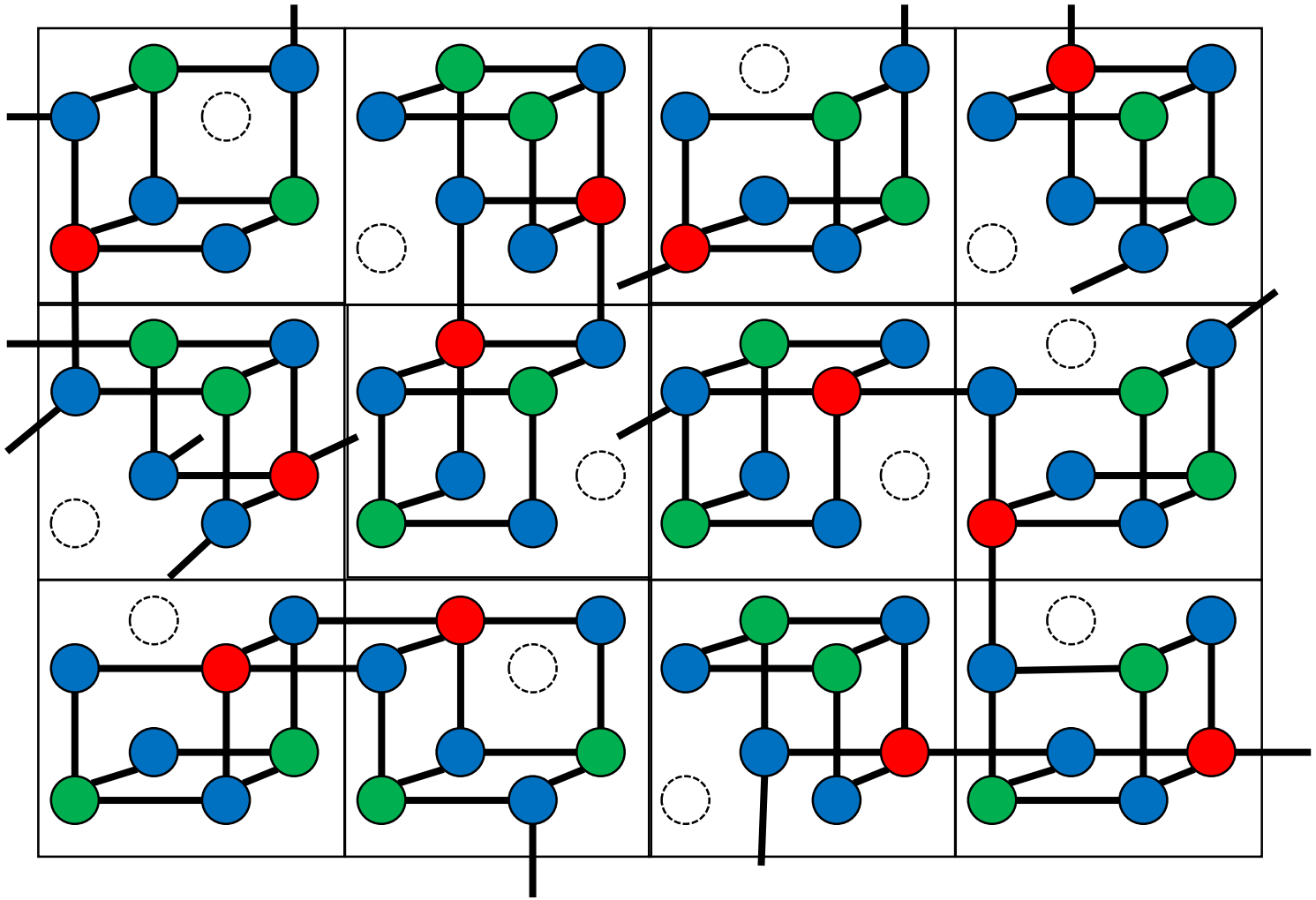


Model of Amorphous structure

In practice, we assume that each unit can rotate and deform its angles and length of bonds such that they are more close to $GeTe_4$ and $SbTe_3$.

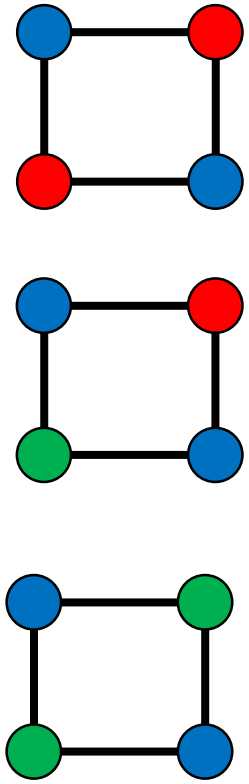
Example:
$(GeTe)(Sb_2Te_3)$

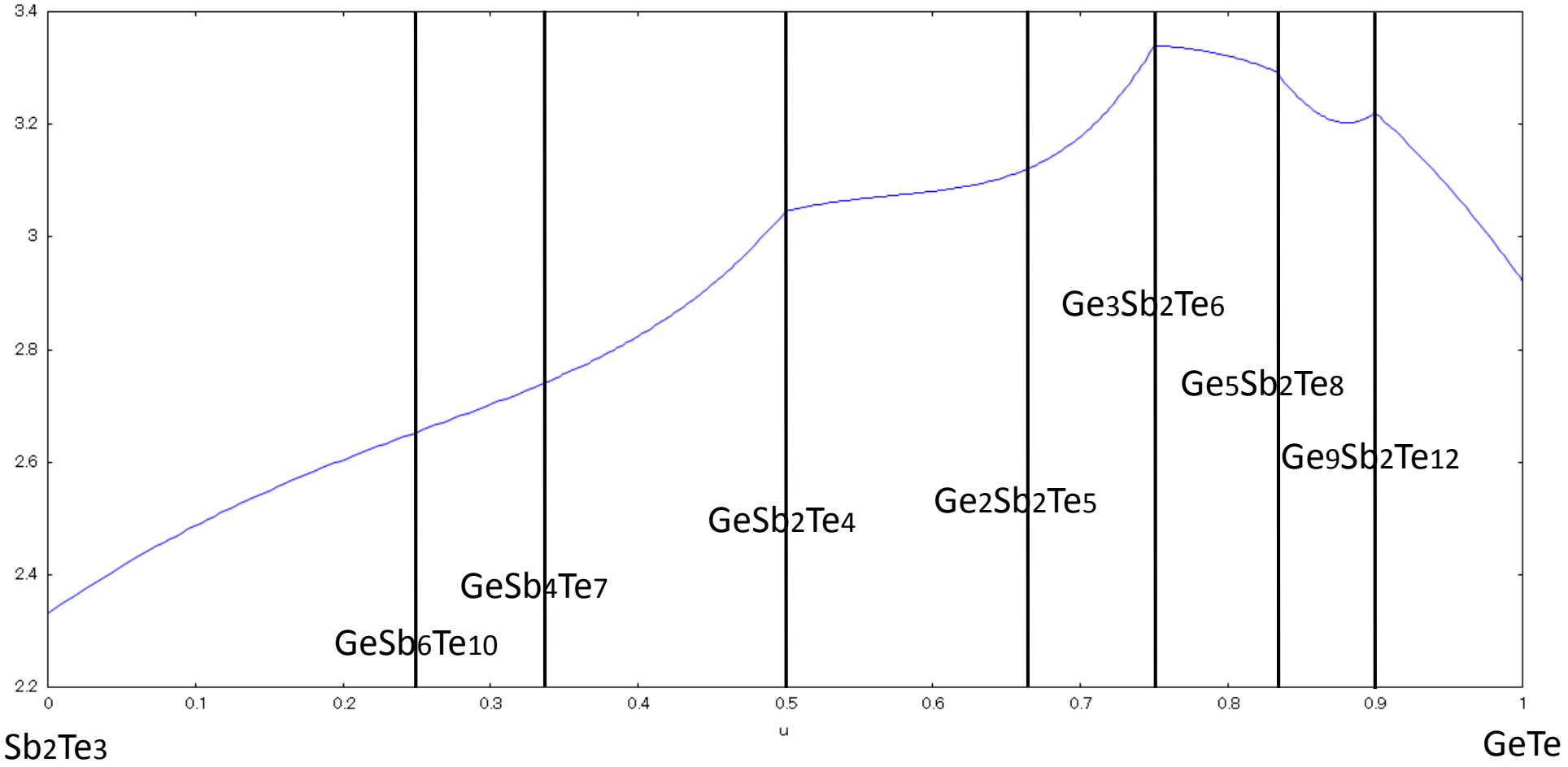




Crystal-like local structure

If the density of 4-membered ring by Ge-Te and Sb-Te in amorphous phase is high, then its local structure may be more crystal-like.

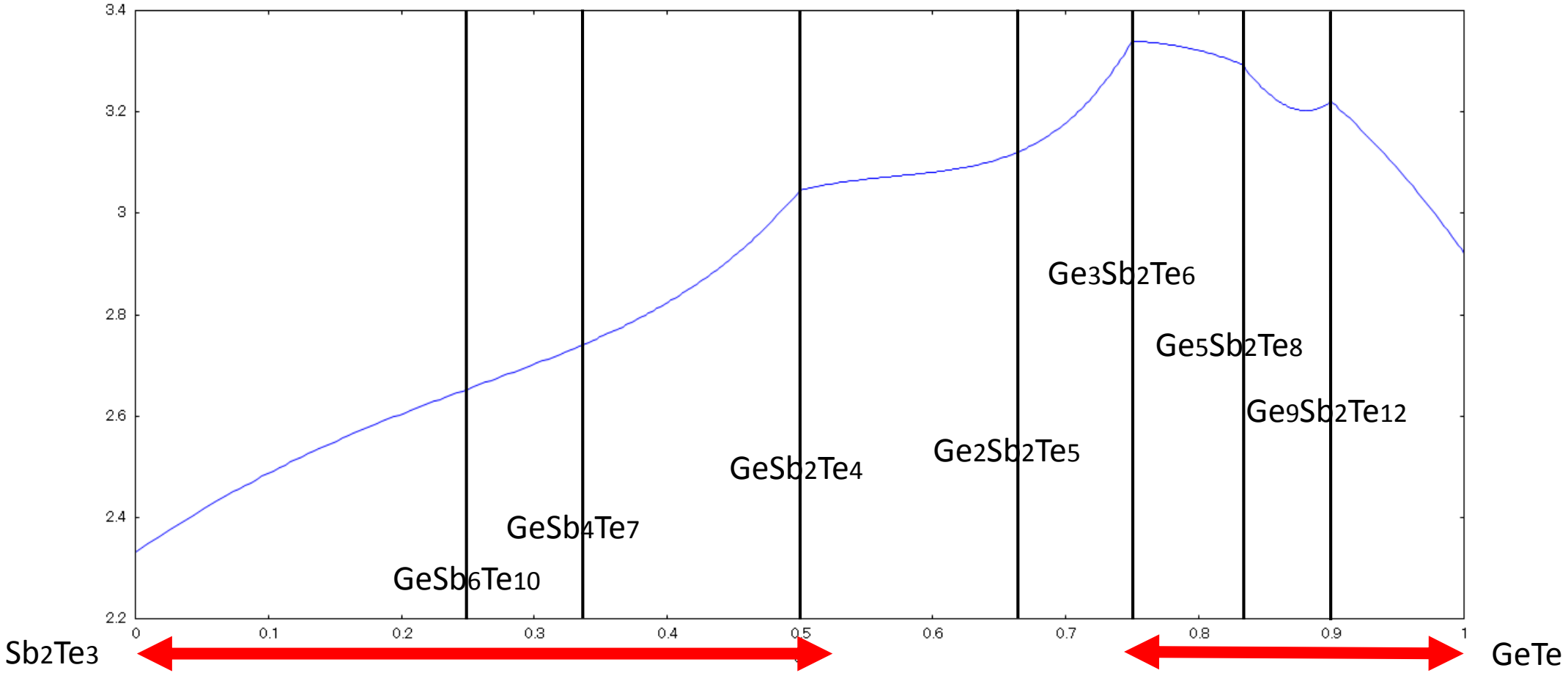




The density of 4-membered ring by Ge-Te and Sb-Te par unit

Global connecting structure

Each atoms are connected by covalent bonds with around atoms.



There are Only Small molecules
by mathematical theorem

Maybe there is Only One Huge molecule
(but we could prove only 2-dim case model)

Summary and future plans

- We gave a model of amorphous structure of GeTe-Sb_2Te_3, which is based on the number of covalent bonds of Ge, Sb, Te, and crystal-like local atomic structure.
- It predicts $Ge_3Sb_2Te_6$ has the most crystal-like local structure. This is on going research, which will be compared with a result by simulation.
- It also predicts that the composition ratio n/m is less than 1 $(GeTe)_n(Sb_2Te_3)_m$, then GeTe-Sb_2Te_3 is an aggregate of small molecules.
- We expect that these results relate to the crystallization temperature and speed.
- This (global structure) model is considered more general situation, and we gave some results as mathematical theorems (see: arXiv:1604.00371)