MedeA Special Quasirandom Structures

Order in Chaos

At-a-Glance

MedeA®[1] *Special Quasirandom Structures* provides quick access to efficient modeling of binaray, ternary, and pseudo-ternary random alloys crystallizing in cubic or hexagonal lattices.

Key Benefits

- Quick access to the most common alloy structures
- Straightforward specification of the alloy composition
- Automated creation of the quasirandom alloy crystal structure

The efficient and at the same time realistic modelling of substitutionally random alloys has been a challenge for very long. For many years, two main kinds of approaches were routinely used. The virtual crystal approximation (VCA) and the coherent potential approximation (CPA) focus on averaging the atomic potentials and the atomic scattering matrices, respectively[2,3], but have difficulties taking local structural distortions into account. Supercell approaches allow a more realistic description, but are computationally demanding, and suffer from limited control of the statistics. Representing alloys as special quasirandom structures (SQS) offers a very elegant solution to this dilemma. The basic idea consists of arranging the different alloying atoms on lattice sites of relatively small unit cells, such that their most relevant radial correlation functions mimic those of a perfectly random structure[4,5]. The validity and usefulness of this approach has been demonstrated in numerous applications for a variety of alloys[6,7,8].

> *Art begins when randomness ends. Although randomness enriches it.*
>
> P. Reverdy, French poet

MedeA Special Quasirandom Structures provides an easy-to-use access to quasirandom structures. As shown in the figure below, it only requires input of the type of alloy, the underlying crystal structure, the lattice parameters, and the types of the constituent atoms. With this minimal information, *MedeA Special Quasirandom Structures* generates a crystal structure, which fulfills the above mentioned requirement of approximating the physically most relevant radial correlation functions of a perfectly random structure.

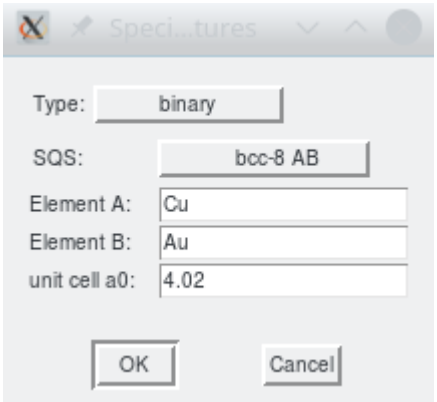

Fig. 1: MedeA Special Quasirandom Structures *screenshot: Graphical user interface for input of the type of alloy, the composition, and the structure of the underlying perfect crystal.*

As an example, a 64-atom structure of a CuAu metal alloy is displayed in the figure below. It was generated by *MedeA Special Quasirandom Structures*, and uses a 2 × 2 × 2 supercell of a face-centered cubic conventional unit cell. Cu and Au

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[2] B. Velicky, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. **175**, 747 (1968) (DOI)

[3] R. J. Elliott, J. A. Krumhansl, and P. L. Leath, Rev. Mod. Phys. **46**, 465 (1974) (DOI)

[4] A. Zunger, S. H. Wei, L. G. Ferreira, and J. E. Bernard, Phys. Rev. Lett. **65**, 353 (1990) (DOI)

[5] S. H. Wei, L. G. Ferreira, J. E. Bernard, and A. Zunger, Phys. Rev. B **42**, 9622 (1990) (DOI)

[6] K. C. Hass, L. C. Davis, and A. Zunger, Phys. Rev. B **42**, 3757 (1990) (DOI)

[7] R. Magri, S. Froyen, and A. Zunger, Phys. Rev. B **44**, 7947 (1991) (DOI)

[8] C. Wolverton and V. Ozolins, Phys. Rev. B **73**, 144104 (2006) (DOI)

atoms are then distributed over the 64 sites following the SQS algorithm.

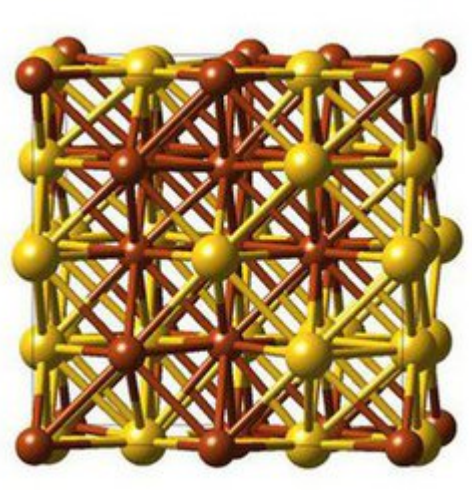

Fig. 2: Crystal structure of CuAu metal alloy as generated by MedeA Special Quasirandom Structures

As another example, a 64-atom structure of an $InGaAs_2$semiconductor alloy, as generated by *MedeA Special Quasirandom Structures*, is shown in the figure below. It is based on $2 \times 2 \times 2$ supercell of the zincblende unit cell. Whereas the As atoms form a regular sublattice, In and Ga atoms are distributed over the other sublattice as determined by the SQS algorithm.

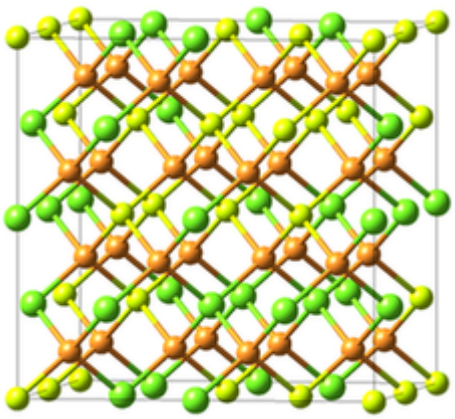

Fig. 3: Crystal structure of an $InGaAs_2$semiconductor alloy as generated by MedeA Special Quasirandom Structures

Key Features

- Straightforward generation of quasirandom crystal structures for binary, ternary, and pseudoternary alloys with face-centered cubic, base-centered cubic or hexagonal close-packed lattices
- Specification of the key ingredients as the underlying ideal structure, as well as the types of the constituent atoms, with an intuitive user interface
- Quasirandom structures generated by *MedeA Special Quasirandom Structures* can be used just like ordered structures, *e.g.* in structure relaxations using *MedeA VASP* or vibrational analysis using *MedeA Phonon*

Properties

- Setup of crystal structures for binary, ternary, and pseudoternary alloys with cubic or hexagonal lattices

Required Modules

- *MedeA Environment*

Related Modules

- *MedeA VASP*
- *MedeA UNCLE*

Find Out More

To learn more about a systematic approach to alloy design using *MedeA's* Universal CLuster Expansion method, check out our datasheet on MedeA UNCLE.

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