Supplementary Information for

Lattice distortion and re-distortion affecting irradiation tolerance in high entropy alloys

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Voronoi tessellation analysis is an effective 3-dimensional (3D) approach to building atomic clusters with one central atom that can be applied for extracting and indexing structural units in complex materials.[1,2] According to Voronoi original algorithm,[3] a convex Voronoi polyhedron (VP) can be built by connecting perpendicular bisectors between a central atom and all of its first-shell neighboring atoms, which may be indexed as <n3, n4, n5, n6…>, where ni denotes the number of i-edged faces on surface of this polyhedron. Each VP should be embedded in a corresponding convex Voronoi cluster (VC), which is composed of a solute (center) atom and its neighboring solvent (shell) atoms (configurations of some VCs and corresponding VPs refer to Fig. 6 in Ref. [2] or Fig. 1 in Ref. [4]). Thus $\sum ni$ also represents the number of the shell atoms in eac VC, i.e., CN parameter around the central atom. Voronoi algorithm also requires that all VCs should be closed structural units, which could be formed by piling up a set of Delaunay tetrahedrons with the common vertex at an atom (the central atom of VC),[5] so that their surface should be composed only of triangle faces, i.e., they could be regarded as deltahedra.[6] Then take into account Euler's formula

$$V - E + F = 2, \tag{1}$$

where V , E and F denote the numbers of vertexes (occupied by atoms), edges and faces of VCs, respectively. V (CN), F and E should satisfy the following equations:

$$3E = 2F = \sum i \times ni$$

$$V = 0.5F + 2. \tag{2}$$

Evidently, $\sum i \times ni$ must be divisible by 6. According to the aforementioned method, various kinds of VCs could be extracted from structural models and correctly indexed.

Supplementary References

[1] J. L. Fenney, *Nature,* 1977, **266,** 309-314.

[2] S. Y. Wang, M. J. Kramer, M. Xu, S. Wu, S. G. Hao, D. J. Sordelet, K. M. Ho and C. Z. Wang, *Phys. Rev. B,* 2009, **79,** 144205.

[3]http://www.ccl.net/cca/software/SOURCES/FORTRAN/allen-tildesley-book/f.35.shtml

[4] L. Yang and G. Q. Guo, *Chin. Phys. B,* 2010, **19,** 126101.

[5] N. N. Medvedev, *J. Comput. Phys.,* 1986, **67,** 223-229.

[6] H. W. Sheng, W. K. Luo, F. M. Alamgir, J. M. Bai and E. Ma, *Nature,* 2006, **439,** 419-425.