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ISSN 2414-3146

Synchrotron powder X-ray diffraction of a refractory high entropy alloy, $Mo_{0.20}Nb_{0.21}Ta_{0.19}V_{0.20}W_{0.20}$

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Received 3 October 2025
Accepted 9 December 2025

Edited by M. Weil, Vienna University of Technology, Austria

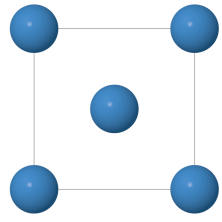
Keywords: powder diffraction; solid solution; high-entropy alloy; refractory metals.

CCDC reference: 2514546

Structural data: full structural data are available from iucrdata.iucr.org

Powder X-ray diffraction data collected at the Advanced Photon Source 16-BM–D, confirms that the alloy with composition $Mo_{0.20}Nb_{0.21}Ta_{0.19}V_{0.20}W_{0.20}$ crystallizes in a simple body-centered cubic (bcc) structure with all five elements distributed over a single crystallographic site (Wyckoff position 2*a* of space group $Im\bar{3}m$).

3D view



Structure description

High-entropy alloys (HEAs) have attracted considerable attention because of their remarkable physical properties and simple crystal structures. Refractory HEAs remain relatively unexplored but are of particular interest for their high melting points and mechanical strength. The title compound, a near equiatomic solid solution with composition $Mo_{0.20}Nb_{0.21}Ta_{0.19}V_{0.20}W_{0.20}$, combines these attributes and has potential for extreme pressure/temperature applications owing to its high shear strength and melting temperature. We report here its crystal structure along with the first publicly available crystallographic information file (CIF) of a refractory HEA (to the best of our knowledge).

Much like the well known Cantor alloy (Cantor *et al.*, 2004), the $Mo_{0.20}Nb_{0.21}Ta_{0.19}V_{0.20}W_{0.20}$ solid solution adopts a simple bcc structure (space group $Im\bar{3}m$), just like the constituent elements themselves. The refined lattice parameter is a = 3.19634 (3) Å, with all constituent elements sharing a single Wyckoff position 2*a* (0, 0, 0) (Fig. 1). The shortest $M—M$ distance and some angles are listed in Table 1. Using the following lattice parameters for individual elements, Mo = 3.147 Å (Ross & Hume-Rothery, 1963), Nb = 3.3004 Å (Straumanis & Zyszczynski, 1970), Ta = 3.38 Å (Srivastava *et al.*, 2011), V = 3.0241 Å (James & Straumanis, 1960), and W = 3.16475 Å (Deshpande & Pawar, 1962), we find that the average elemental lattice parameter is $\langle a \rangle$ = 3.20325 Å and therefore the difference relative to the title compound is 0.22%. With such a small

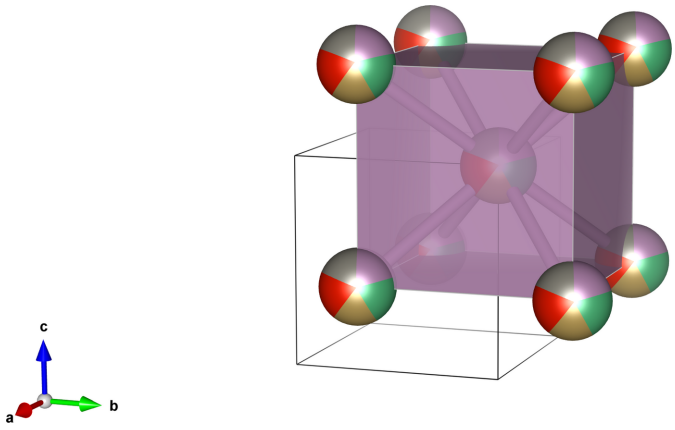


Figure 1
The first nearest neighbors coordination formed around the 2*a* site with coordination number 8; the different colors represent the fractional occupancies.

difference from the mean we report that Vegard's law holds for this solid solution (Denton & Ashcroft, 1991). The elemental and high-entropy alloy lattice parameters along with the arithmetic mean of the constituent elements are shown in Fig. 2.

Synthesis and crystallization

Elemental powders of Mo, Nb, Ta, V, and W (nominal purity >99.9%) were weighed in equiatomic proportions and mixed thoroughly to achieve homogeneity. The mixture was pressed into a pellet and placed into the chamber of a MAM-1 vacuum arc-melter (Edmund Bühler GmbH, Bodelshausen, Germany). The chamber was evacuated and then pumped with argon to ensure an inert atmosphere. The pellet was then melted at approximately 3500 K and cooled rapidly on a water-cooled copper hearth yielding a dense, single-phase ingot. The ingot was then powdered in a mortar and pestle until particle size was below 5 microns.

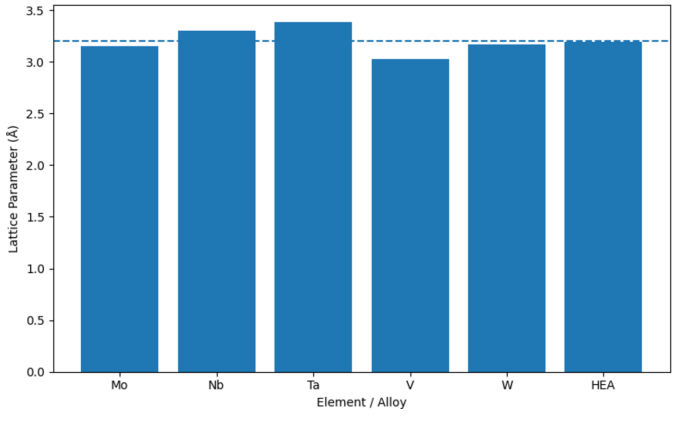


Figure 2
The elemental and high-entropy alloy lattice parameters along with the arithmetic mean of the constituent elements as a dashed line.

Table 1
Selected geometric parameters (Å, °).

Mo3—Mo3^{i}	2.7681 (3)		
Mo3^{i}—Nb2—Mo3^{ii}	70.529	Mo3^{i}—Nb2—Mo3^{iii}	109.471

Symmetry codes: (i) $x-\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (ii) $x-\frac{1}{2}, y-\frac{1}{2}, z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$Mo_{0.20}Nb_{0.21}Ta_{0.19}V_{0.20}W_{0.20}$
M_r	120.04
Crystal system, space group	Cubic, $Im\overline{3}m$
Temperature (K)	300
a (Å)	3.19634 (3)
V (Å^3)	32.66 (1)
Z	2
Radiation type	Synchrotron, Advanced Photon Source, 16-BM-D, λ = 0.42460 Å
μ (mm^{-1})	28.17
Specimen shape, size (mm)	Irregular, 0.0015 × 0.0015
Data collection	
Diffractometer	Local diffractometer set-up
Specimen mounting	Ambient sample holder on Kapton tape
Data collection mode	Transmission
Scan method	Step
2θ values (°)	$2\theta_{min}$ = 2.737 $2\theta_{max}$ = 33.372 $2\theta_{step}$ = 0.020
Refinement	
R factors and goodness of fit	R_p = 0.266, R_{wp} = 0.388, R_{exp} = 0.563, $R(F^2)$ = 0.27811, χ^2 = 0.476
No. of parameters	1

Computer programs: *EPICS* (Mooney *et al.*, 1996), *GSAS-II* (Toby & Von Dreele, 2013), *DIOPTAS* (Prescher & Prakapenka, 2015) and *VESTA* (Momma & Izumi, 2008), *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection, and structure refinement details can be found in Table 2. Synchrotron powder X-ray diffraction

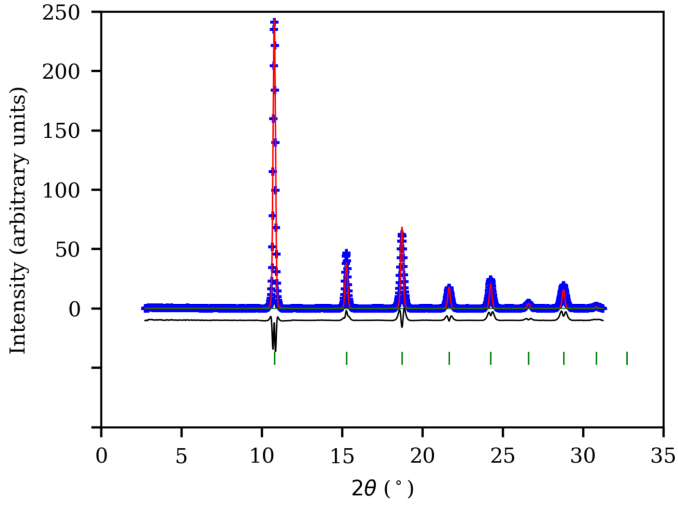


Figure 3
Rietveld difference plot for the single-phase refinement of $Mo_{0.20}Nb_{0.21}Ta_{0.19}V_{0.20}W_{0.20}$. The blue crosses show the observed data, the red line the calculated data and the gray line the difference plot. Calculated Bragg reflection positions are indicated by green tick marks.

data were processed using *DIOPTAS* (Prescher & Prakapenka, 2015) and analyzed *via* Rietveld refinement in *GSAS-II* (Toby & von Dreele, 2013). A single crystallographic site was used for all five elements; their fractional occupancies were constrained to sum to unity during refinement, as determined by energy dispersive spectroscopy, using a Quanta 650 FEG scanning electron microscope (see supplementary figure). Isotropic displacement parameters for all elements were held fixed at the default *GSAS-II* value and not refined. Since there are five different atoms on a single Wyckoff site, refining this lead to unphysical values. It should be noted that the rather high reliability factors of the Rietveld refinement (Fig. 3) probably are due to the standard uncertainties being overestimated (Toby, 2006).

Acknowledgements

This material is based upon work supported by the Department of Energy-National Nuclear Security Administration Center of Excellence CAMCSE under Award Number DE-NA0004154. Portions of this work were performed at HPCAT (Sector 16), Advanced Photon Source (APS), Argonne National Laboratory. HPCAT operations are supported by DOE's NNSA's Office of Experimental Sciences. The Advanced Photon Source is a U.S. Department of Energy (DOE) Office of Science user facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. The calculations utilized the National Energy Research Scientific Computing Center (NERSC), a U.S. DOE Office of Science User Facility, supported under Contract No. DE-AC02-05CH11231, using NERSC Award BES-ERCAP0033090.

References

Cantor, B., Chang, I. T. H., Knight, P. & Vincent, A. J. B. (2004). *Mater. Sci. Eng. A* **375–377**, 213–218.
Denton, A. R. & Ashcroft, N. W. (1991). *Phys. Rev. A* **43**, 3161–3164.
Deshpande, V. T. & Pawar, R. (1962). *Curr. Sci.* **31**, 497.
James, W. J. & Straumanis, M. E. (1960). *J. Electrochem. Soc.* **107**, 69.
Momma, K. & Izumi, F. (2008). *J. Appl. Cryst.* **41**, 653–658.
Mooney, T. M., Cha, B. K., Goetze, K. A., Reid, D. R. & Winans, J. R. (1996). *Rev. Sci. Instrum.* **67**, 3369–3372.
Prescher, C. & Prakapenka, V. B. (2015). *High Pressure Res.* **35**, 223–230.
Ross, R. G. & Hume-Rothery, W. (1963). *J. Less-Common Met.* **5**, 258–270.
Srivastava, A., Chauhan, M. & Singh, R. K. (2011). *Phys. Status Solidi B* **248**, 2793–2800.
Straumanis, M. E. & Zyszczynski, S. (1970). *J. Appl. Cryst.* **3**, 1–6.
Toby, B. H. (2006). *Powder Diffr.* **21**, 67–70.
Toby, B. H. & Von Dreele, R. B. (2013). *J. Appl. Cryst.* **46**, 544–549.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2025). **10**, x251109 [https://doi.org/10.1107/S2414314625011095]

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Molybdenum niobium tantalum vanadium tungsten

Crystal data

$Mo_{0.20}Nb_{0.21}Ta_{0.19}V_{0.20}W_{0.20}$
M_r = 120.04
Cubic, $Im\bar{3}m$
Hall symbol: -I423
a = 3.19634 (3) Å
V = 32.66 (1) Å^3
Z = 2
D_x = 12.208 Mg m^{-3}

Synchrotron, Advanced Photon Source, 16-BM-D radiation, λ = 0.42460 Å
μ = 28.17 mm^{-1}
T = 300 K
gray metallic
irregular, 0.002 × 0.002 mm
Specimen preparation: Prepared at 3500 K

Data collection

Local
diffractometer set-up
Specimen mounting: Ambient sample holder on Kapton tape

Data collection mode: transmission
Scan method: step
$2\theta_{min}$ = 2.737°, $2\theta_{max}$ = 33.372°, $2\theta_{step}$ = 0.020°

Refinement

Least-squares matrix: full
R_p = 0.266
R_{wp} = 0.388
R_{exp} = 0.563
$R(F^2)$ = 0.27811
1505 data points

Profile function: Finger-Cox-Jephcoat function parameters U, V, W, X, Y, SH/L: peak variance(Gauss) = Utan(Th)^2+Vtan(Th)+W: peak HW(Lorentz) = X/cos(Th)+Ytan(Th); SH/L = S/L+H/L U, V, W in (centideg)^2, X & Y in centideg 1.163, -0.126, 50.000, 0.000, 6.864, 0.002,
1 parameters
0 restraints
0 constraints
Weighting scheme based on measured s.u.'s
$(\Delta/\sigma)_{max}$ < 0.001
Background function: Background function: "chebyschev-1" function with 3 terms: 0.059, 0.001, 0.094,
Preferred orientation correction: March-Dollase correction coef. = 1.000 axis = [0, 0, 1]

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Mo3	0.00000	0.00000	0.00000	0.0250*	0.2000

Nb2	0.00000	0.00000	0.00000	0.0250*	0.2100
Ta1	0.00000	0.00000	0.00000	0.0250*	0.1900
V1	0.00000	0.00000	0.00000	0.0250*	0.2000
W4	0.00000	0.00000	0.00000	0.0250*	0.2000

Geometric parameters (Å, º)

Mo3—Mo3^{i}	2.7681 (3)		
Mo3^{i}—Nb2—Mo3^{ii}	70.529	Mo3^{i}—Nb2—Mo3^{iii}	109.471

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