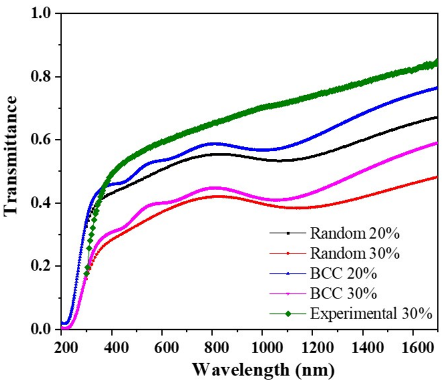

Fig. 2. Comparison of FDTD (*bcc* and random particle distribution) and experimental transmittance. FDTD used bulk Mo optical parameters and metal volume fraction f=20% and 30%.

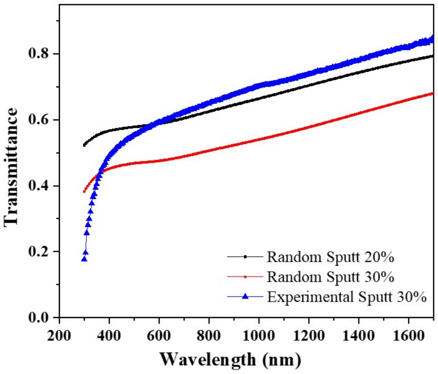

Fig. 4. Comparison of FDTD (random particle distribution) and experimental transmittance. FDTD used optical parameters of sputter Mo and metal volume fraction f=20% and 30%.

fractions (f): i) body centric cubic (*bcc*) lattice arrangement and ii) random distribution of the nanoparticles. In all cases, we assumed a monodisperse distribution with the diameter of 2 nm based on the TEM analysis results. This has been proved to be a good approximation when particle diameter is considerably smaller than the wavelength of the incident radiation [3]. In the case of *bcc* lattice, we changed the value of f by changing the distance between particles around 3 nm. Fig. 1 shows the comparison between the experimental reflectance and FDTD reflectance calculated using the optical parameters for bulk Mo metal volume fraction f=20% and 30%. We observe that the experimental reflectance is better fitted for f = 20%, for both random and *bcc* cases. The random case is very similar to the *bcc* case, but with a less prominent broad dip. The reflectance minimum is much better described for the *bcc* case. For the transmittance shown in Fig. 2, we also have the best fit for f =20%. We note that the behavior of transmittance at low wavelengths is well described for FDTD simulations using bulk Mo optical parameters. Fig. 3 and 4, present the effect of the optical parameters extracted for sputtered Mo on the FDTD calculated reflectance and transmittance. In the case of reflectance, the agreement between the curves is remarkable for f = 20%, except that the reflectance minimum in the measured spectrum is not well reproduced as the calculated one. This discrepancy may be stemmed from the fact that the disorder considered in the particle positions or the optical properties of Mo nanoparticles are not accurately defined in the simulations. In the case of transmittance, we observe a good fit above 500 nm. The discrepancy below 500 nm can be related to the same effect in the case of reflectance minimum or the inaccuracy of the optical parameters used for Mo, which were calculated using the experimental spectral of a sputtered Mo thin film. The optical properties of Mo nanoparticles in our nanocomposite non-necessarily present the same optical properties as a sputtered Mo film.

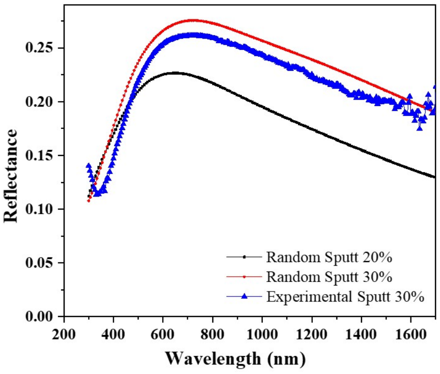

Fig. 3. Comparison of FDTD (random particle distribution) and experimental reflectance. FDTD used optical parameters of sputter Mo and metal volume fraction f=20% and 30%.

IV. CONCLUSION

We have shown that FDTD simulations can accurately predict the reflectance and transmittance of sputtered Mo-Al_2O_3 nano composites even with the strict monodisperse assumption. The results show that use of experimentally obtained optical parameters for Mo significantly improves the accuracy of the simulations. We have also observed that use of random particle distribution considerably improves the accuracy of the calculated R and T spectra, but some characteristics as such as reflectance minimum are better reproduced using *bcc* particle arrangement. The presented results can help designing more efficient solar selective absorbers.

ACKNOWLEDGEMENT

This work was partially supported by Army Research Laboratory (ARL) Multiscale Multidisciplinary Modeling of Electronic Materials Collaborative Research Alliance (Grant No. W911NF-12-2-0023, PM: Dr. M. L. Reed).

REFERENCES

[1] J. Y. Lu, A. Raza, N. X. Fang, G. Chen, and T. Zhang, “Effective dielectric constants and spectral density analysis of plasmonic nanocomposites,” *J. Appl. Phys.*, vol. 120, no. 16, p. 163103, Oct. 2016.

[2] M. R. Nejati, V. Fathollahi, and M. K. Asadi, “Computer simulation of the optical properties of high-temperature cermet solar selective coatings,” in *Solar Energy*, 2005, vol. 78, no. 2, pp. 235–241.

[3] C. Etrich, S. Fahr, M. Keshavarz Hedayati, F. Faupel, M. Elbahri, and C. Rockstuhl, “Effective Optical Properties of Plasmonic Nanocomposites,” *Materials (Basel).*, vol. 7, pp. 727–741, 2014.

[4] M. D. Thoreson, “Fabrication and realistic modeling of three-dimensional metal-dielectric composites,” *J. Nanophotonics*, vol. 5, no. 1, p. 051513, Jan. 2011.

[5] C. Helgert *et al.*, “Effective properties of amorphous metamaterials,” *Phys. Rev. B*, vol. 79, no. 23, p. 233107, Jun. 2009.

[6] “Nanophotonic FDTD Simulation Software - Lumerical FDTD.” [Online]. Available: https://www.lumerical.com/products/fdtd/. [Accessed: 08-Apr-2020].