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Overcoming the trade-off between curing temperature and conductivity for high-performance conductive silver pastes

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Silver powders with three different sizes have been used to form a face-centered cubic (FCC) lattice. The packing density of an FCC arrangement is 0.7405. The first silver powder has a diameter of 25.17 μm, 74.05% of the total volume is occupied under FCC dense packing condition. The selection of the second type of silver powder is listed below:

1 In octahedral voids

The maximum radius of a sphere that can be accommodated within an octahedral void is determined by multiplying the silver powder particle radius by a factor of 0.414. Specifically, for silver powder with a diameter of 25.17 μm (radius of 12.59 μm), the maximum sphere radius is calculated as follows:

$$r_{\max} = 12.59\ \mu\text{m} \times 0.414 = 5.2123\ \mu\text{m} \quad \text{(S1)}$$

Therefore, the maximum radius of silver powder particles within the octahedral voids is 5.2123 μm. When silver powder particles with this radius are used to fill the octahedral voids, the packing density is calculated using the following equation:

$$\text{Packing ratio} = \frac{\frac{4}{3}\pi \times (5.2123)^3 \times 4}{\left(25.17\sqrt{2}\right)^3} = 0.05258 \quad \text{(S2)}$$

2 In tetrahedral voids

Similarly, the maximum radius of a sphere that can be accommodated within a tetrahedral void is calculated by multiplying the silver powder particle radius by a factor of 0.225. For silver powder with a diameter of 25.17 μm (radius of 12.59 μm), the maximum sphere radius in tetrahedral voids is:

$$r_{\max} = 12.59 \times 0.225 = 2.8328\ \mu\text{m} \quad \text{(S3)}$$

Thus, the maximum radius of silver powder particles within the tetrahedral voids is 2.8328 μm. The packing density for spherical silver powder with a radius of 2.8328 μm is calculated as follows:

$$\text{Packing ratio} = \frac{\frac{4}{3}\pi \times (2.8328)^3 \times 8}{(25.17\sqrt{2})^3} = 0.01688 \quad \text{(S4)}$$

3 Packaging ratio after adding the second type of silver powder

Combining the two aforementioned filling modes, the selection of the second type of silver powder must account for the effective filling of voids in both stacking configurations. Consequently, the second type of silver powder should comprise two distinct particle sizes, specifically with the maximum radii of 5.2123 and 2.8328 μm, respectively, which results in a cumulative packing ratio of:

$$0.05258 + 0.01688 = 0.06946 \quad \text{(S5)}$$

However, commercially available silver powders typically do not precisely meet such specific size requirements. To address this limitation, we selected spherical silver powder with a radius ranging from 2.5 to 6.0 μm and an average radius of 4.98 μm.

Based on the calculations derived from the ideal silver powder aggregation model, spherical silver powders with a radius of R_1 = 12.59 μm occupy 74.05% of the total volume, spherical silver powders with a radius of R_2 = 4.98 μm occupy 6.946% of the total volume, and spherical silver powders with a radius of R_3 = 0.095 μm occupy no more than 19.004% of the total volume.

4 XRD pattern of surface oxidized silver powder

The XRD pattern of the surface oxidized silver was shown in Fig. S1. High-temperature oxidation method was used for surface oxidation of silver nanoparticles. Silver nanoparticles were treated in a tube furnace under controlled conditions: the temperature was set to 300 °C with a gas mixture of 30 vol.% oxygen and 70 vol.% nitrogen. The furnace was heated to the target temperature at a rate of 5 °C·min^{-1} and maintained under isothermal conditions for 3 h. Characteristic peaks of Ag_2O at 2θ of approximately 32.8°, 38.1°, 54.9°, and 65.5° correspond to (111), (200), (220), and (311) planes, respectively. All these peaks are absent in the silver powder used in the paper, which indicates that the surface oxidation is negligible.

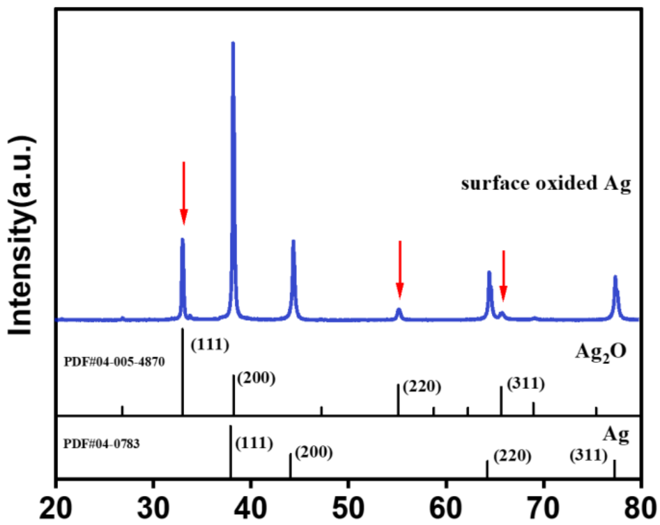

Fig. S1 XRD pattern of surface oxidized silver powder.