

Supporting Information

Growth mechanism for the controlled synthesis of MgH_2/Mg crystals via a vapor-solid process

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- (4) Figure S4: Mg gas condensation rate and the hydrogenation rate for solidified Mg at 1 and 2 MPa H_2 , respectively.

Figure S1

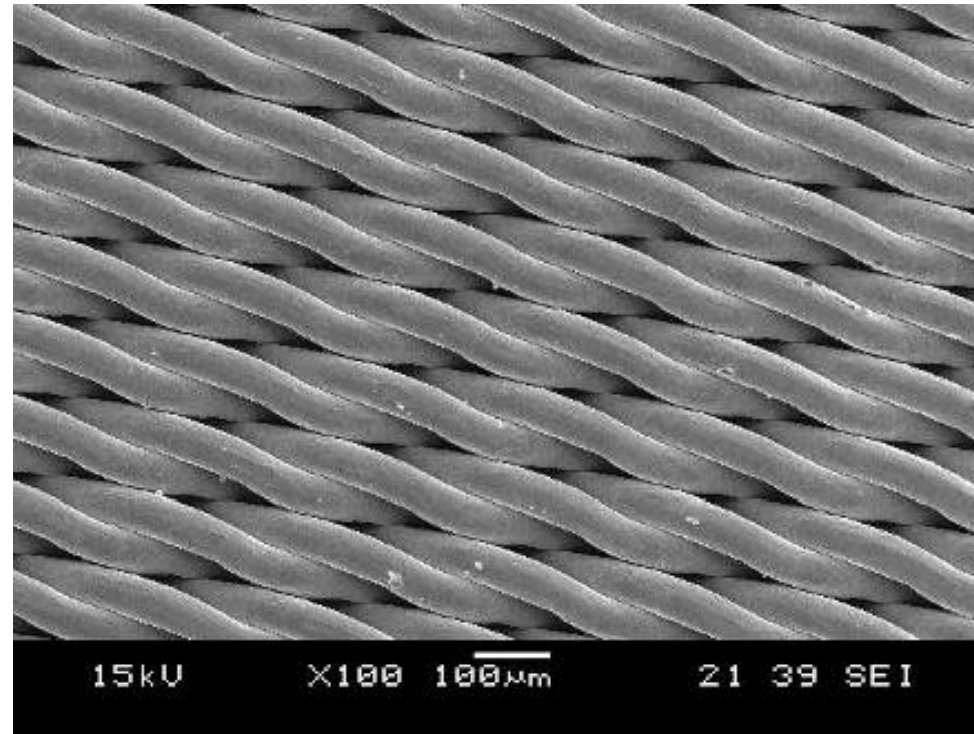


Figure S1. The enlarged image of the mesh (SUS316) used to collect the products in this study.

Figure S2 – (1). 1 MPa product image

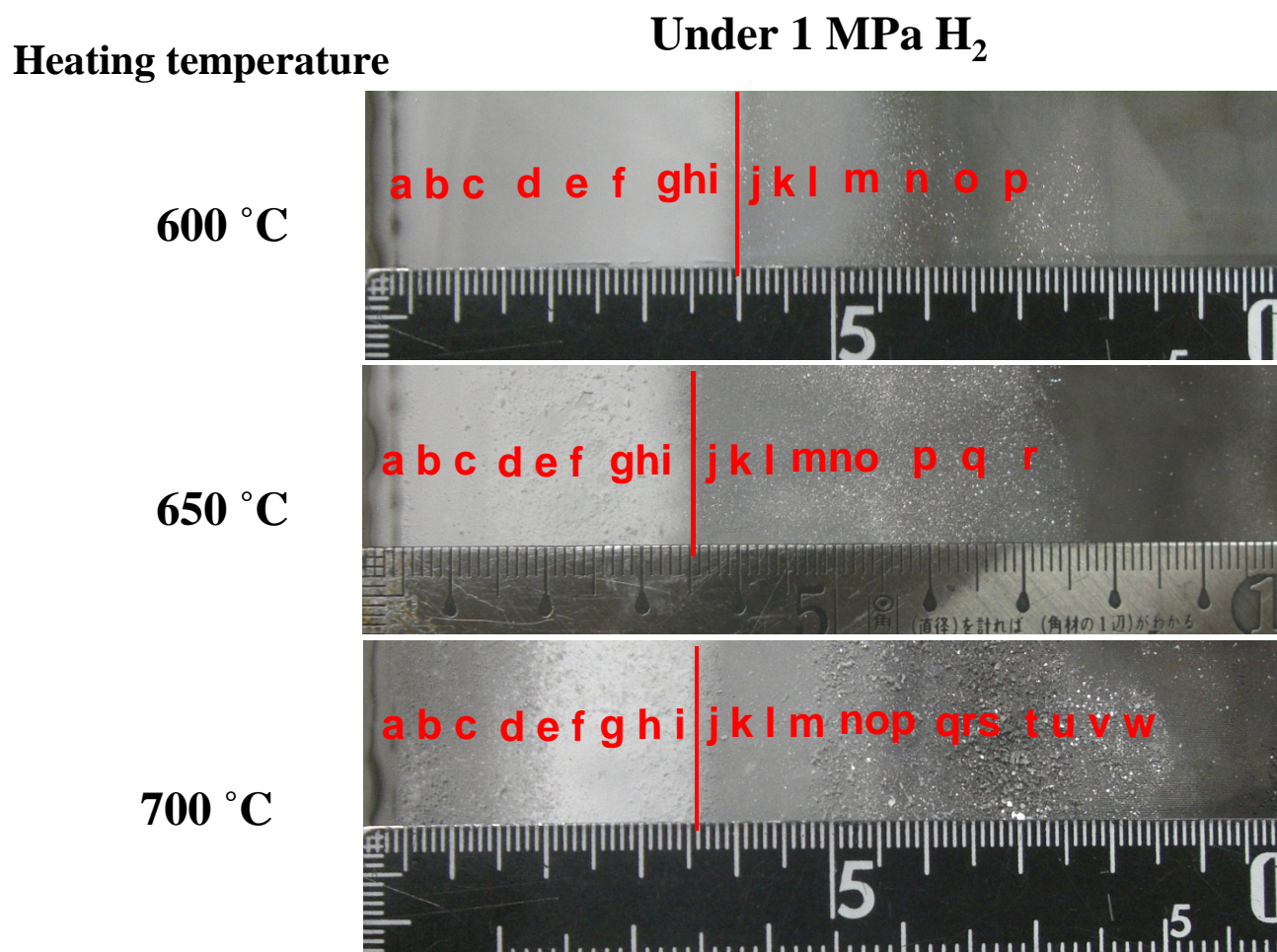


Figure S2 – (1). The images of the product obtained at 1 MPa H₂ with evaporation temperatures of 600, 650, and 700 °C. The abc... numbers are for SEM observation.

Figure S2 – (2). 1 MPa temperature distribution

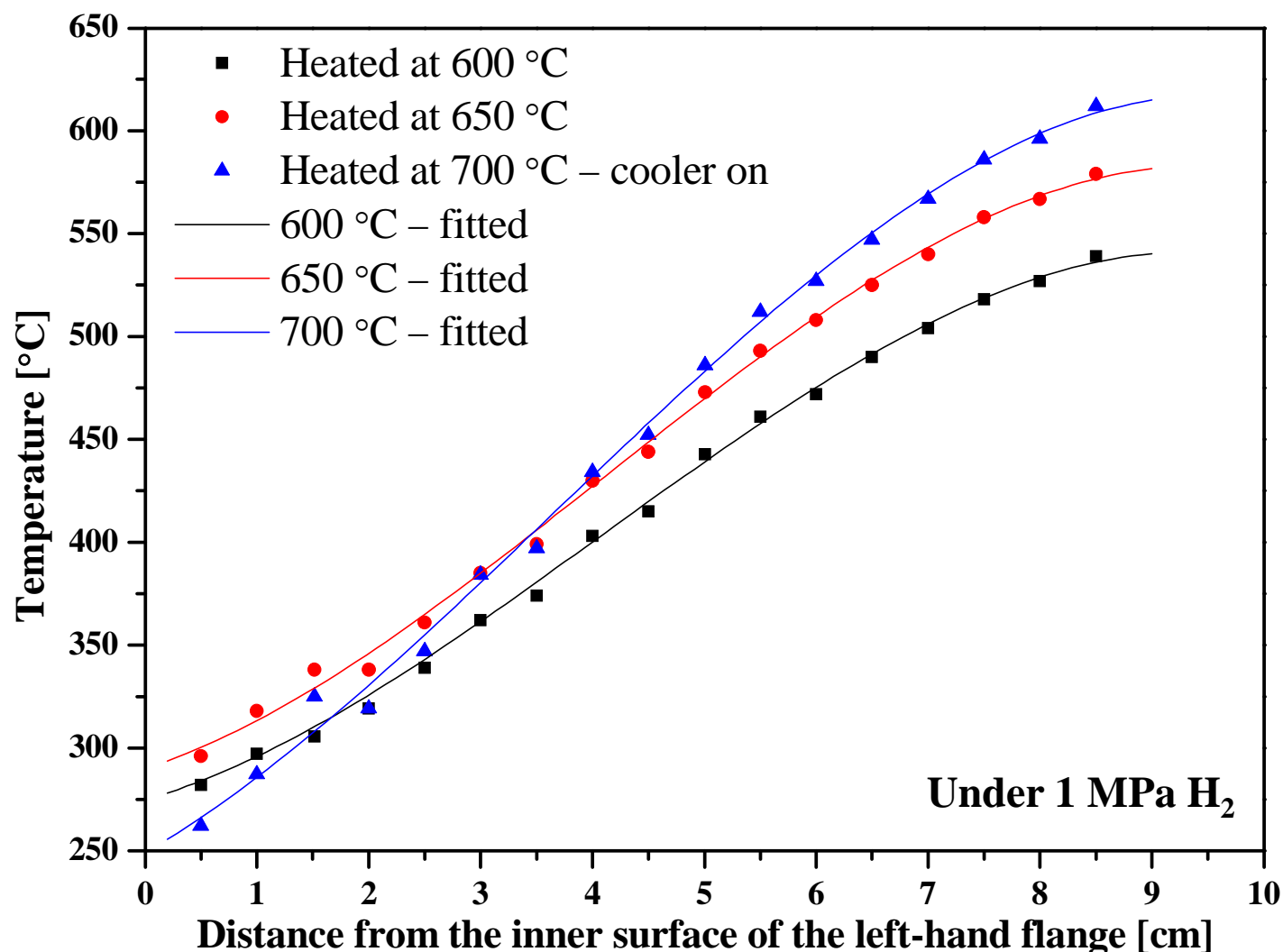
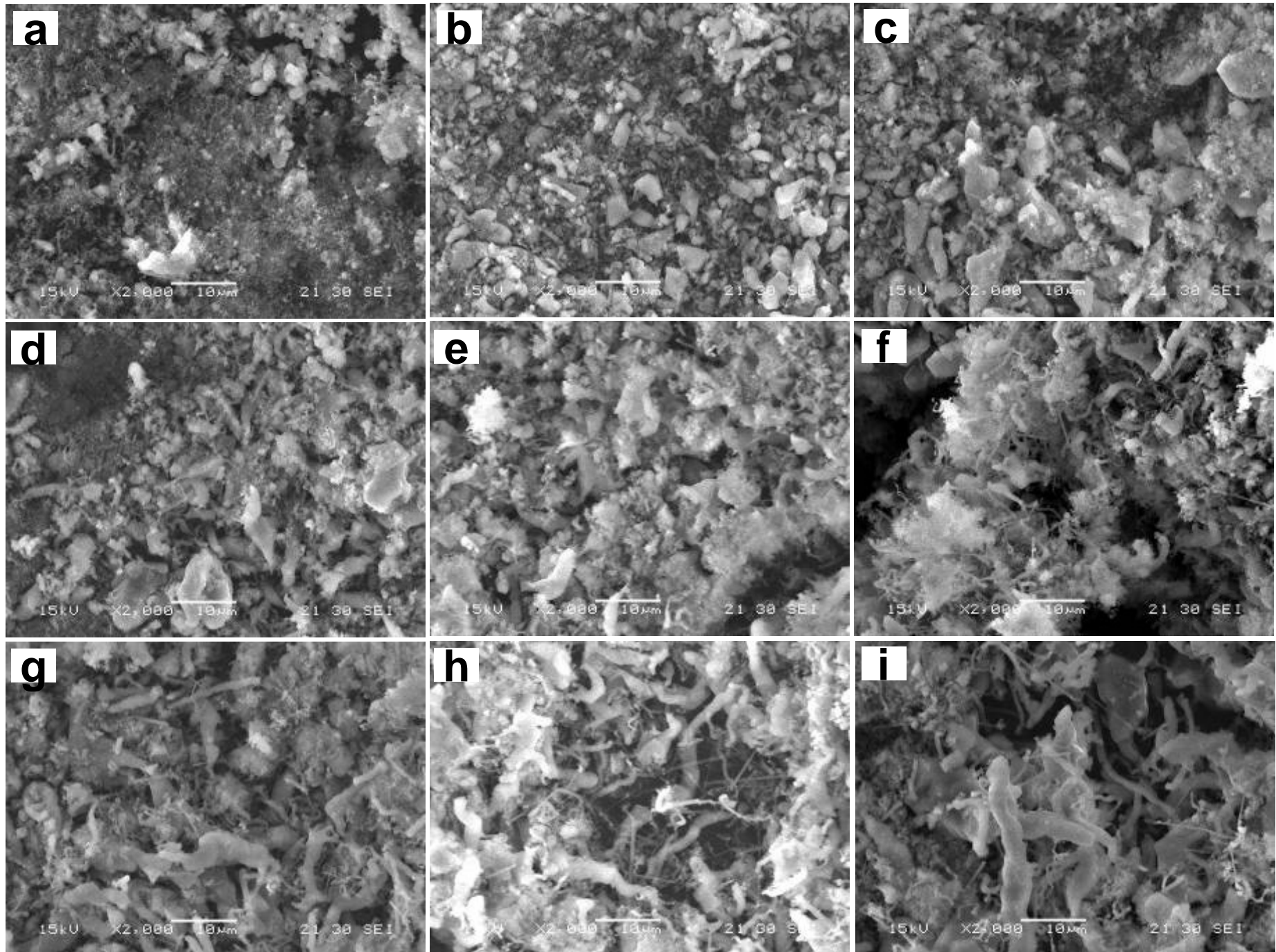


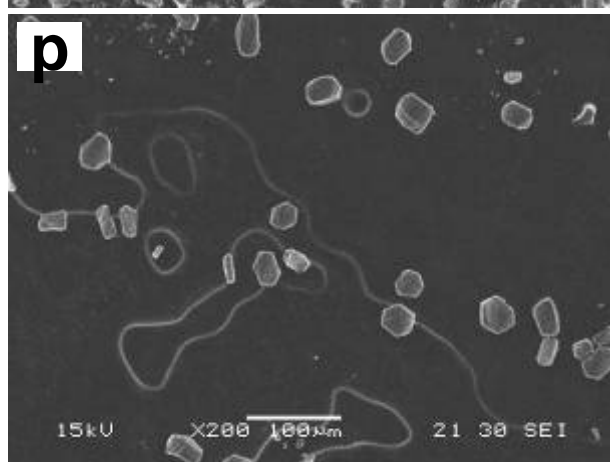
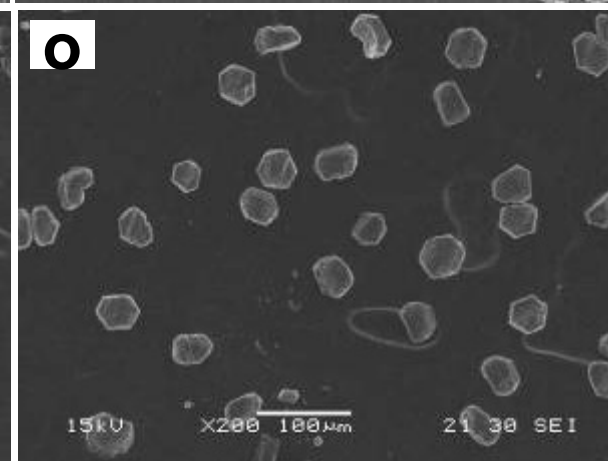
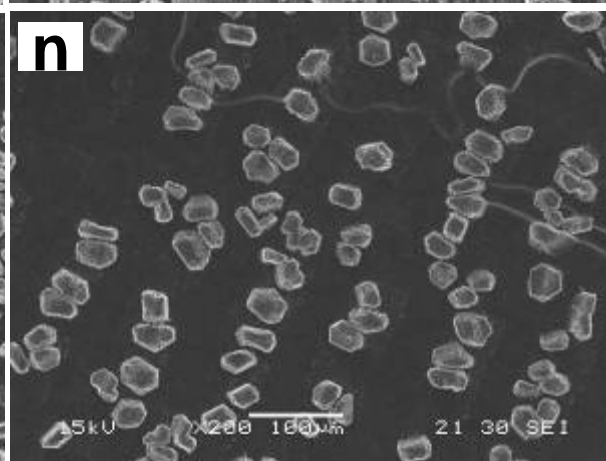
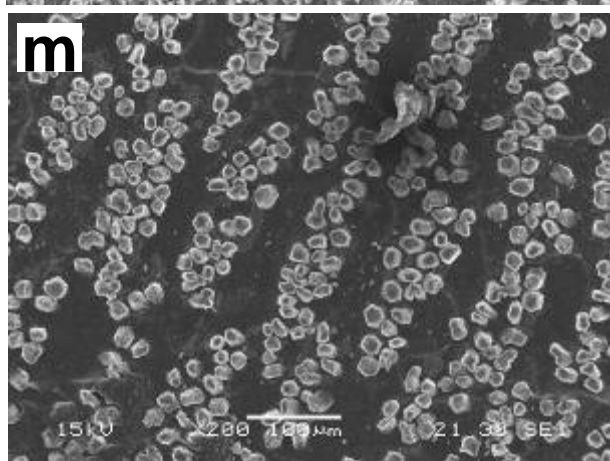
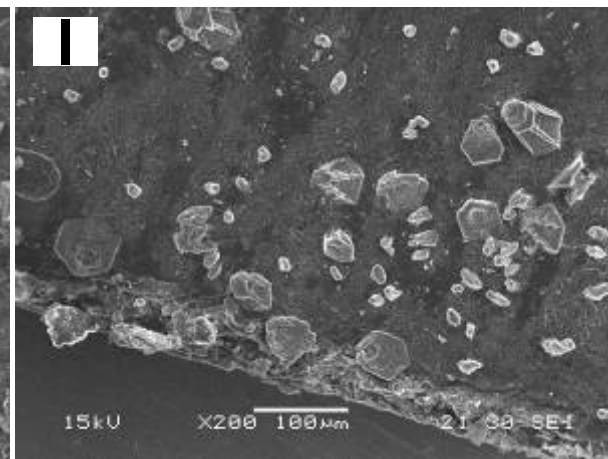
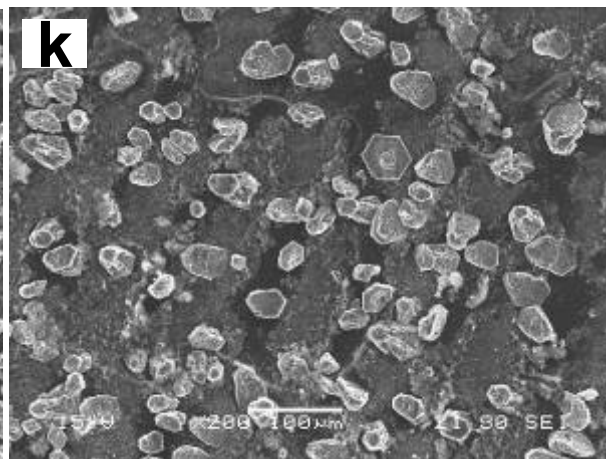
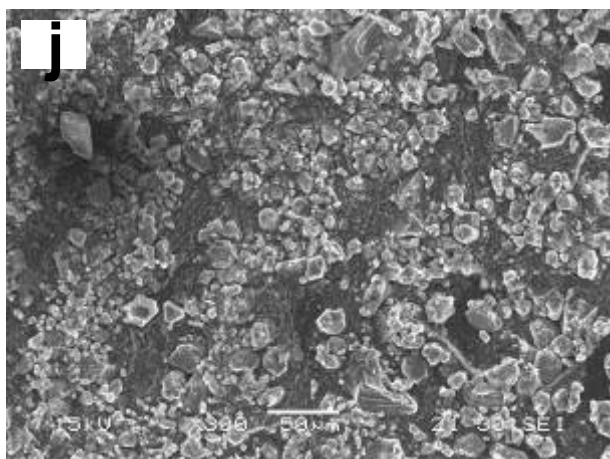
Figure S2 – (2). Temperature distribution on the mesh adhered along the tube wall under 1 MPa H₂ pressure at different evaporation temperatures. To make sure that the lowest deposition temperature is below 300 °C, a cooler jacket was set around the flange with a evaporation temperature of 700 °C.

Figure S2 – (3). 1 MPa SEM images

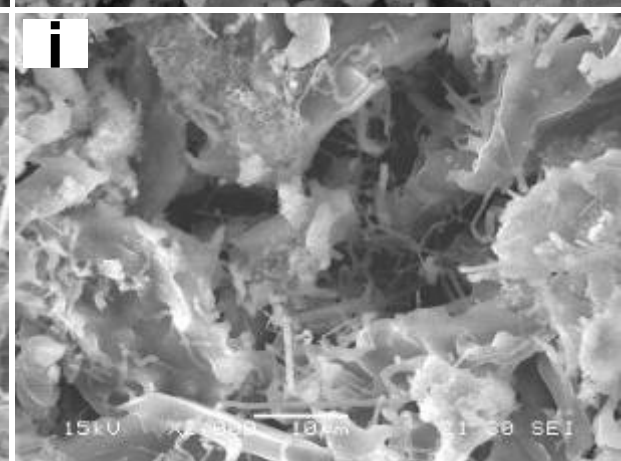
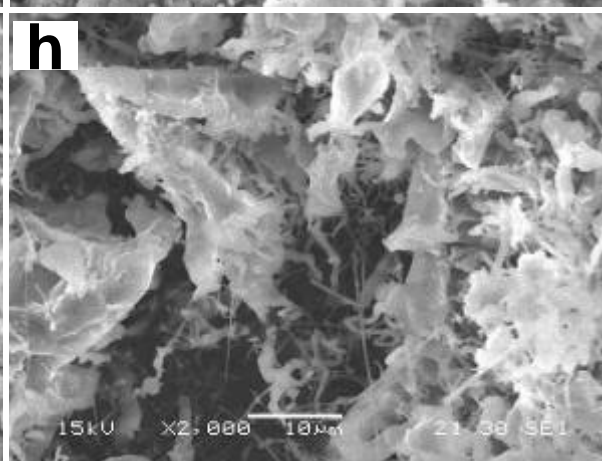
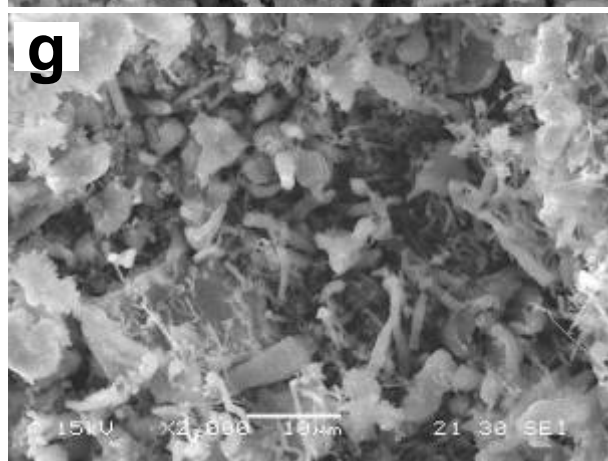
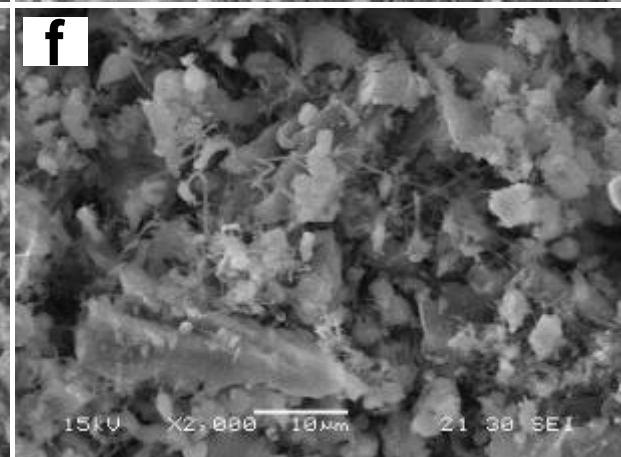
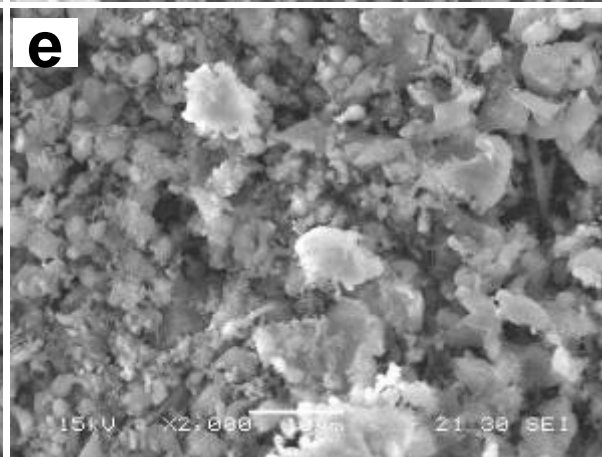
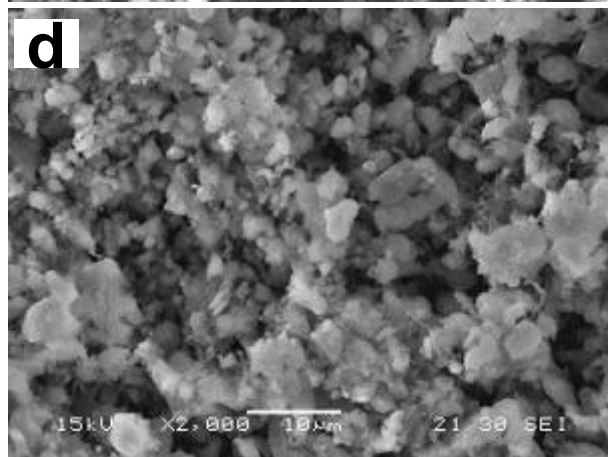
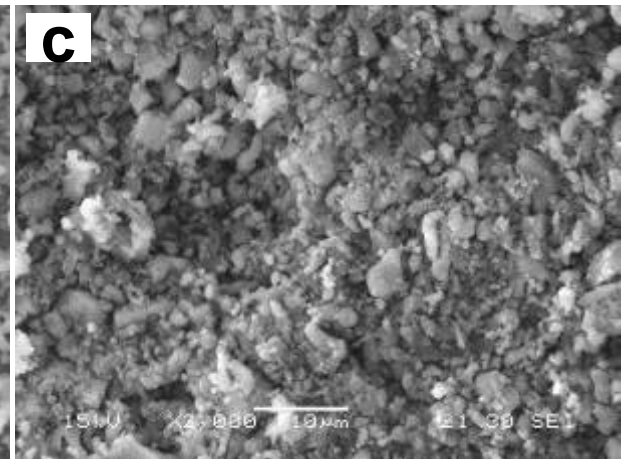
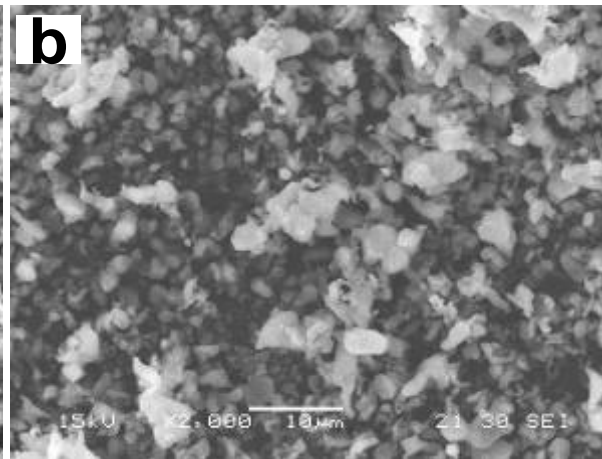
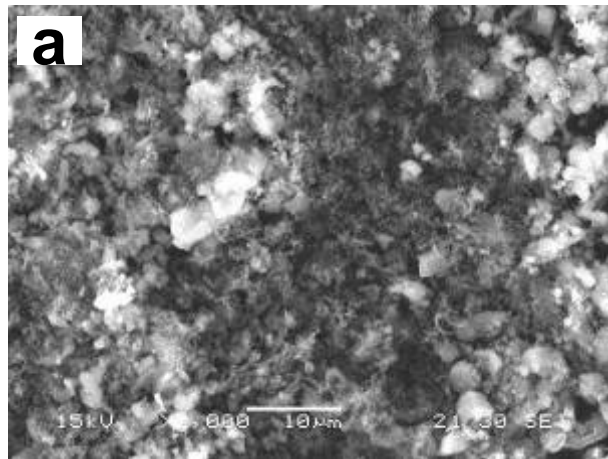
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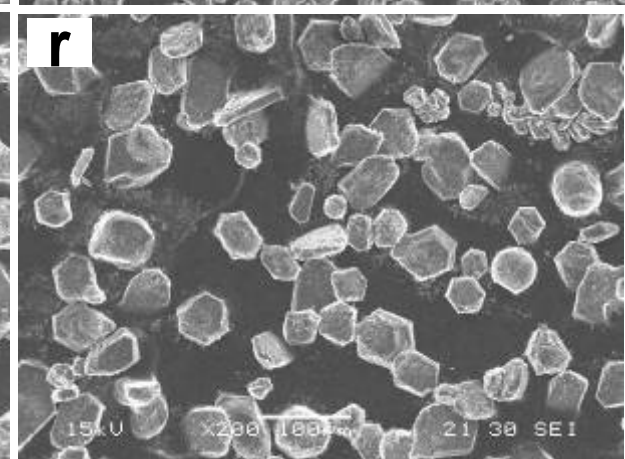
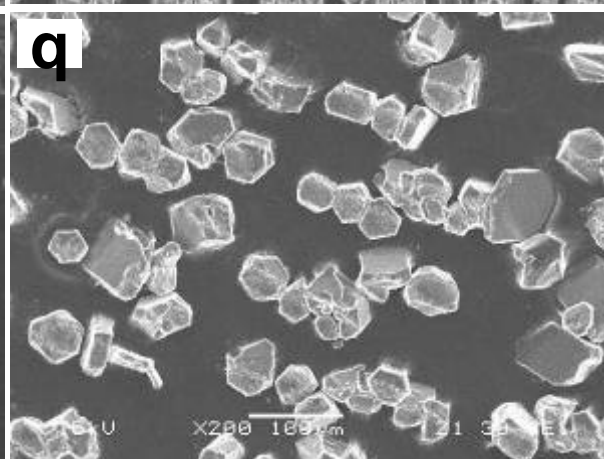
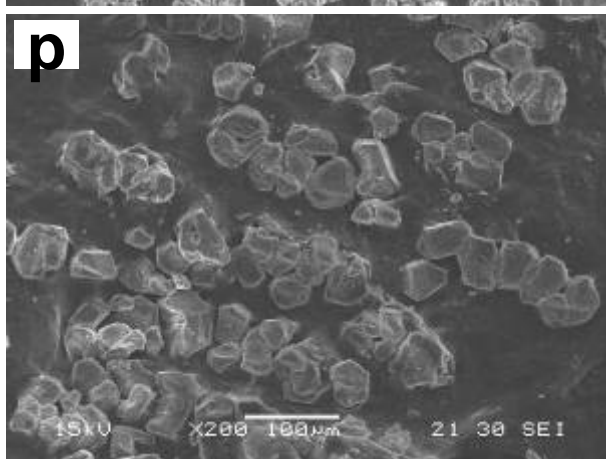
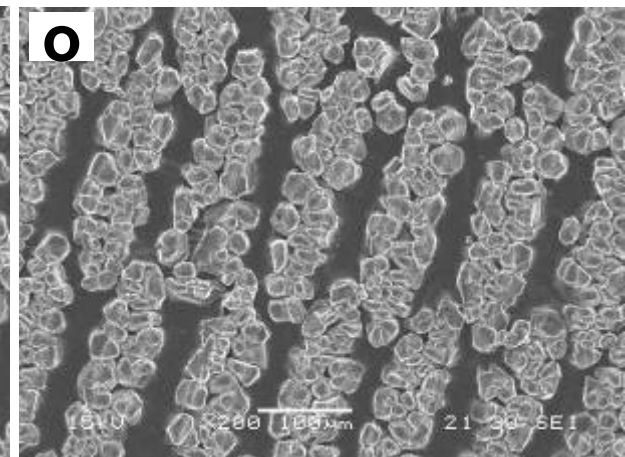
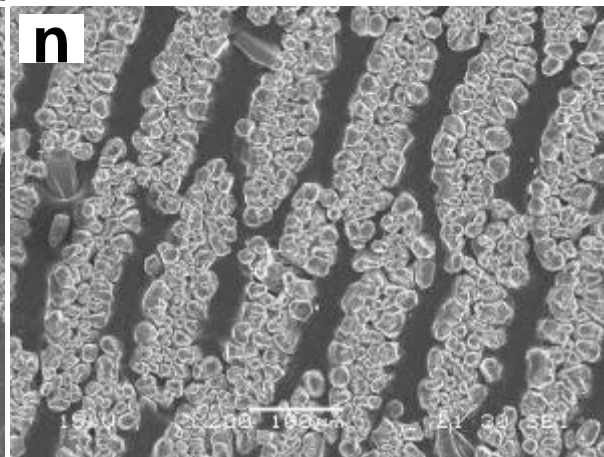
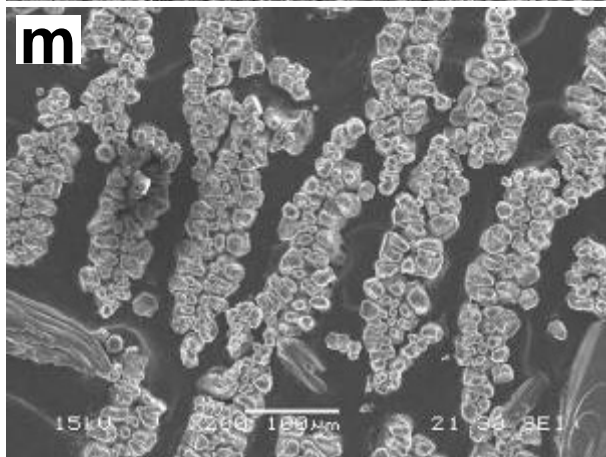
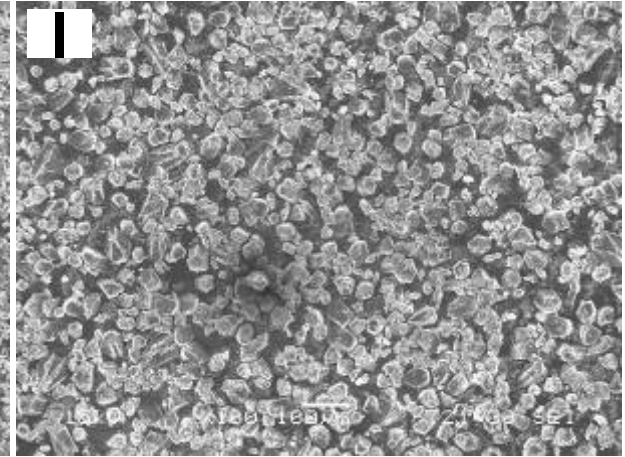
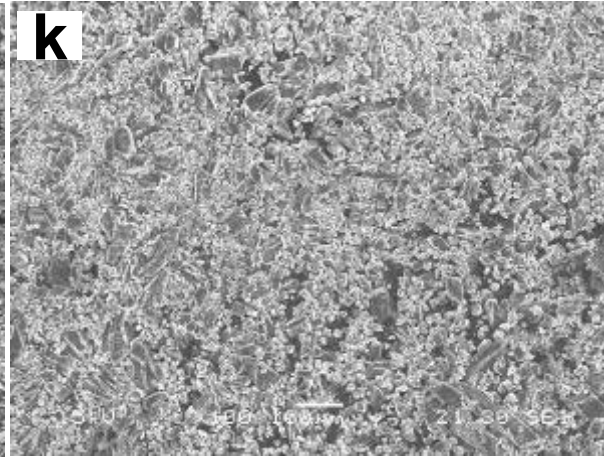
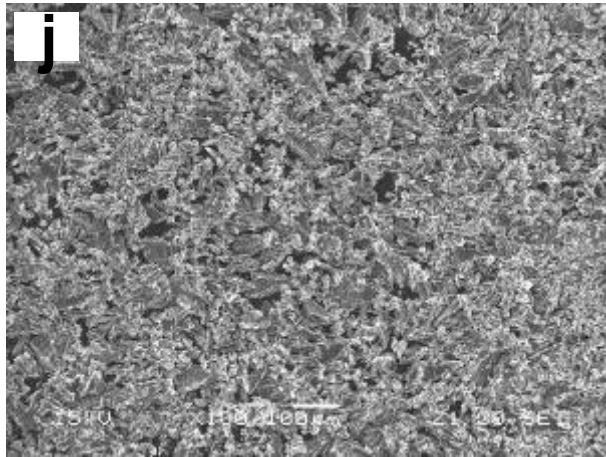
1 MPa-600 °C



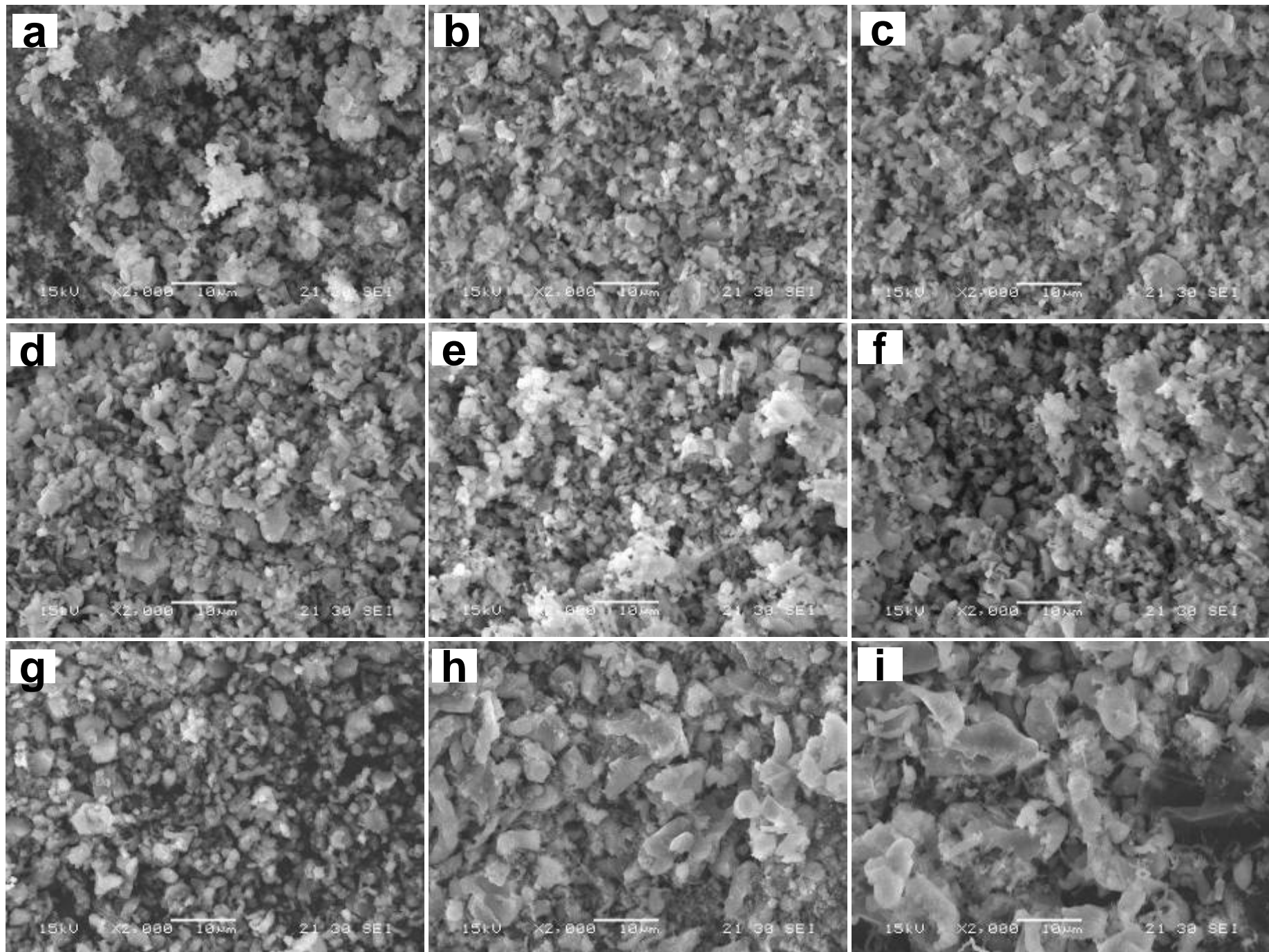
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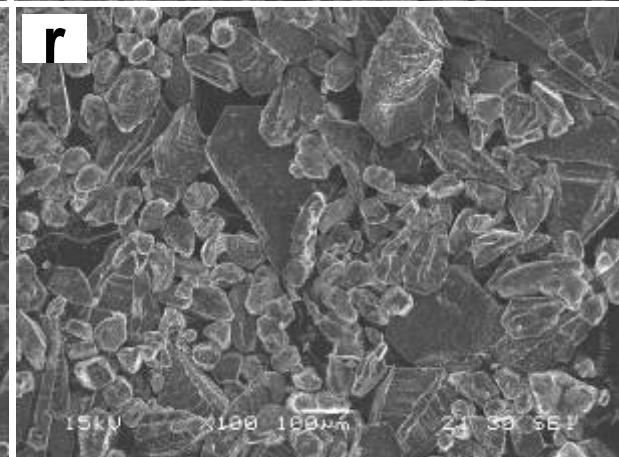
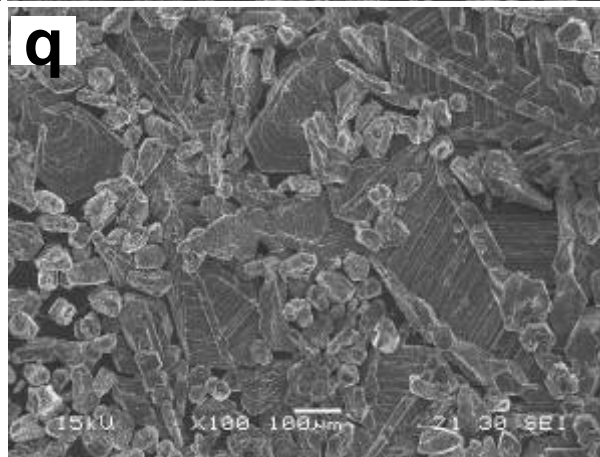
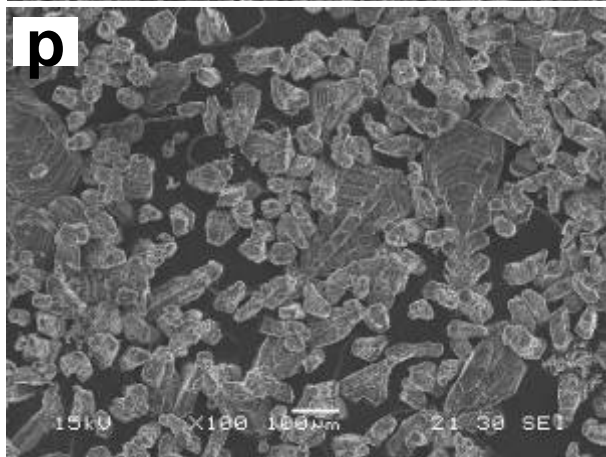
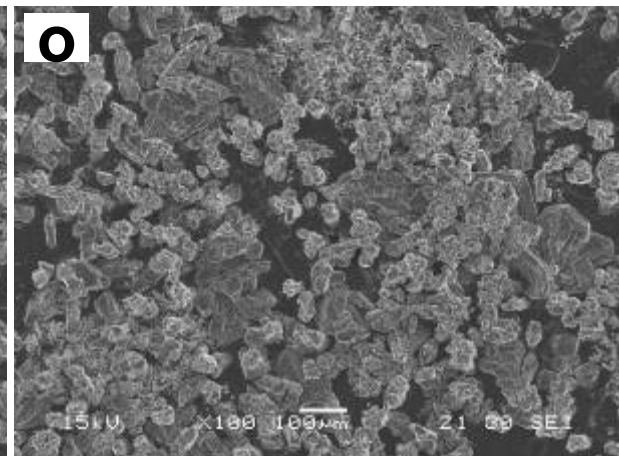
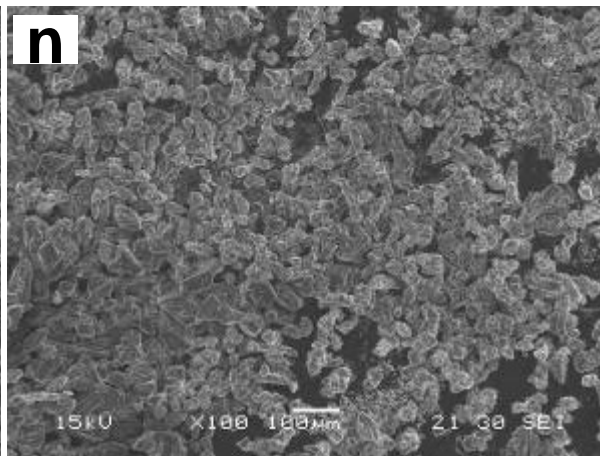
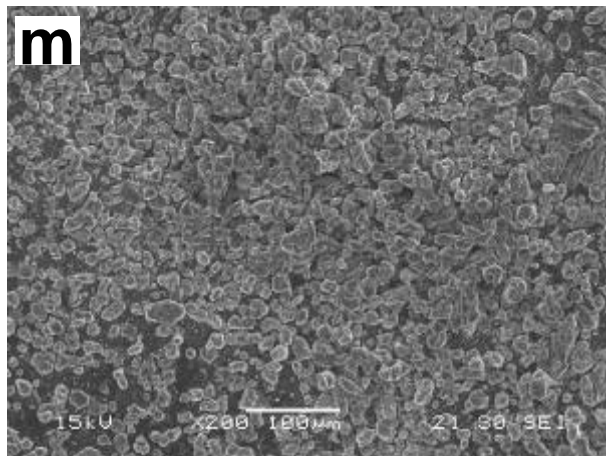
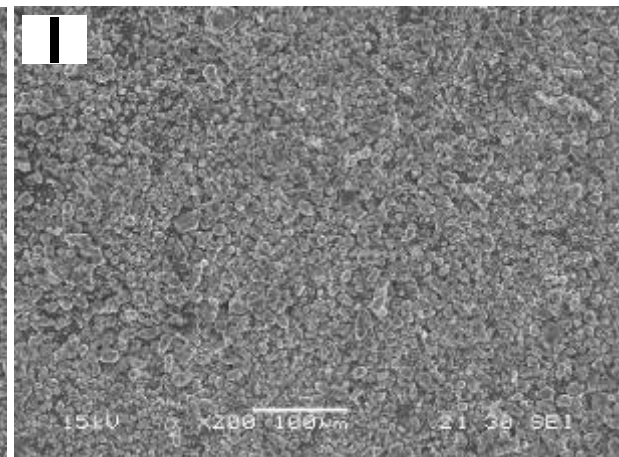
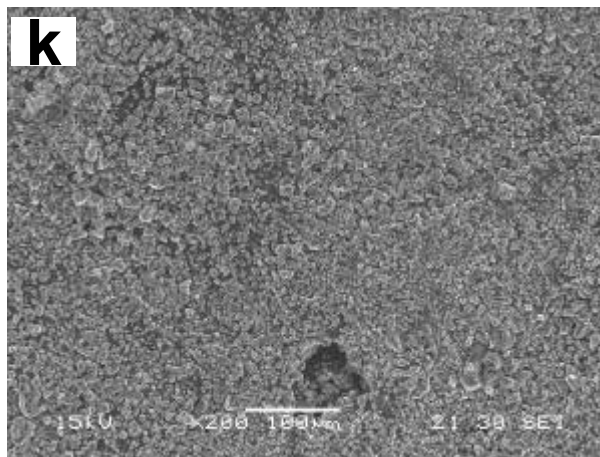
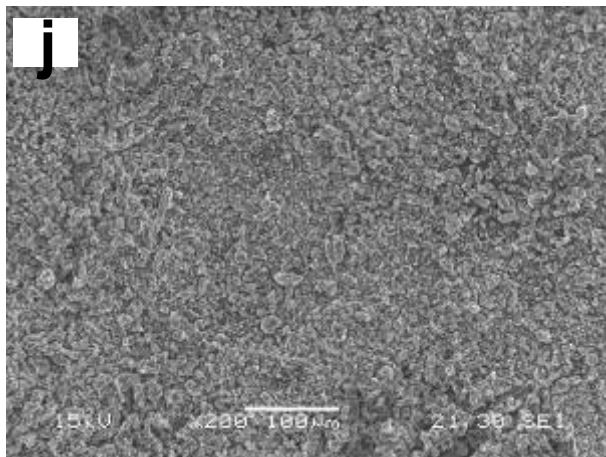
1 MPa-650 °C



1 MPa-700 °C



1 MPa-700 °C



1 MPa-700 °C

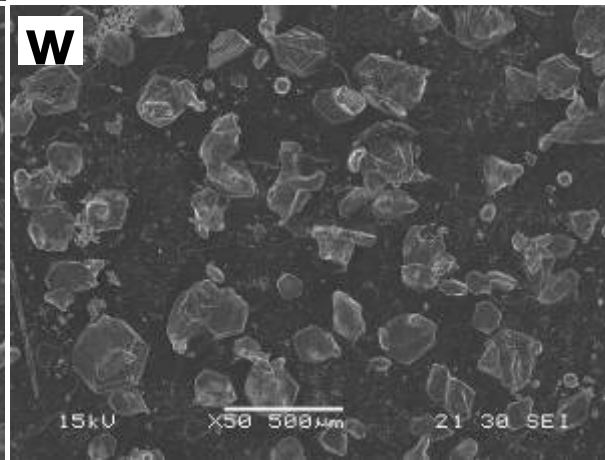
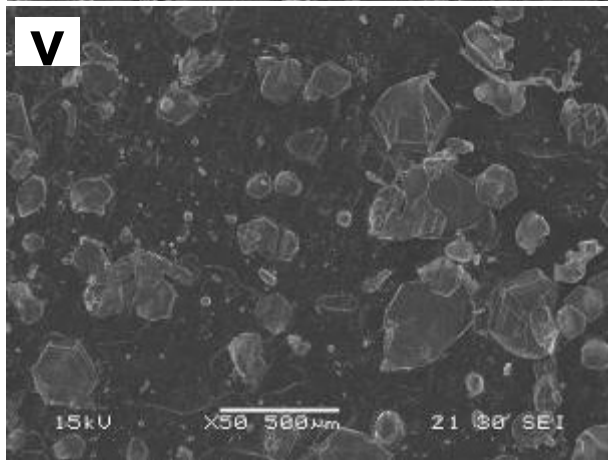
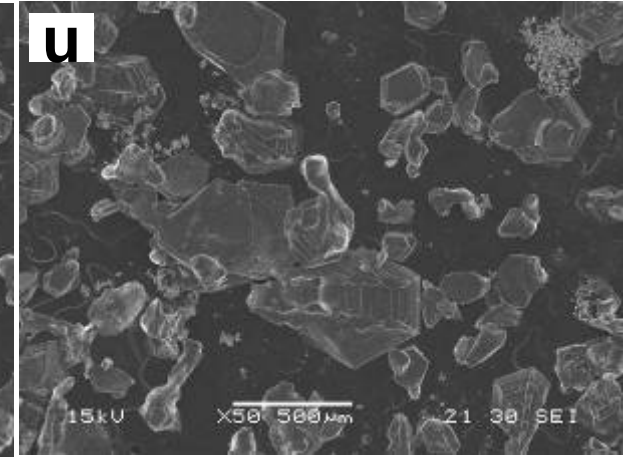
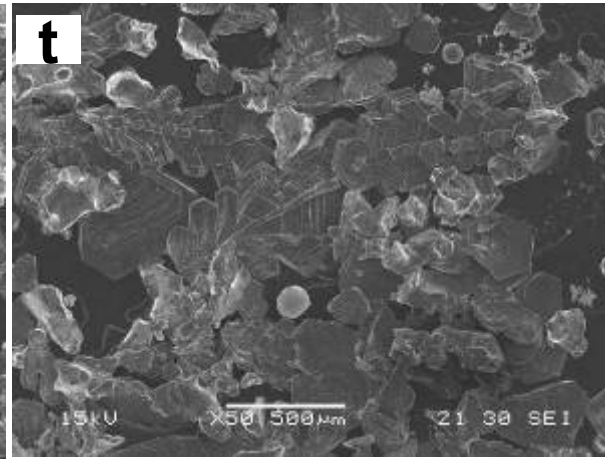
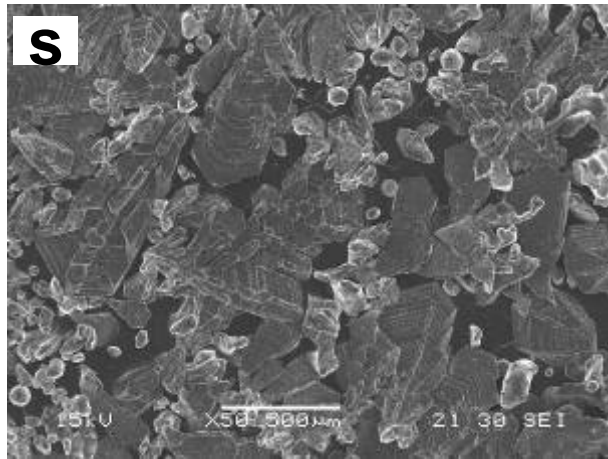


Figure S3 – (1). 2 MPa product image

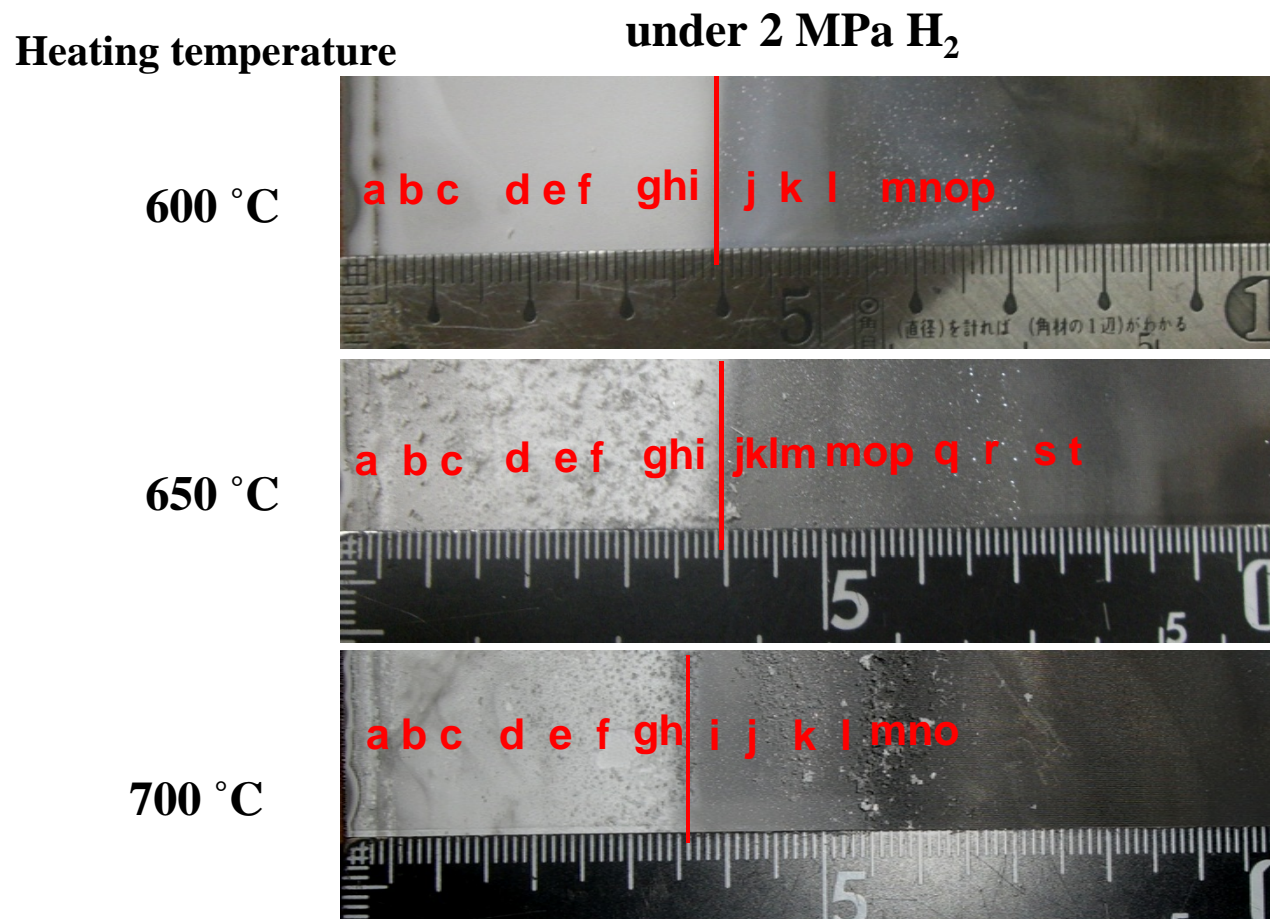


Figure S3 – (1). The images of the product obtained at 2 MPa H₂ with evaporation temperatures of 600, 650, and 700 °C. The abc... numbers are for SEM observation.

Figure S3 – (2). 2 MPa temperature distribution

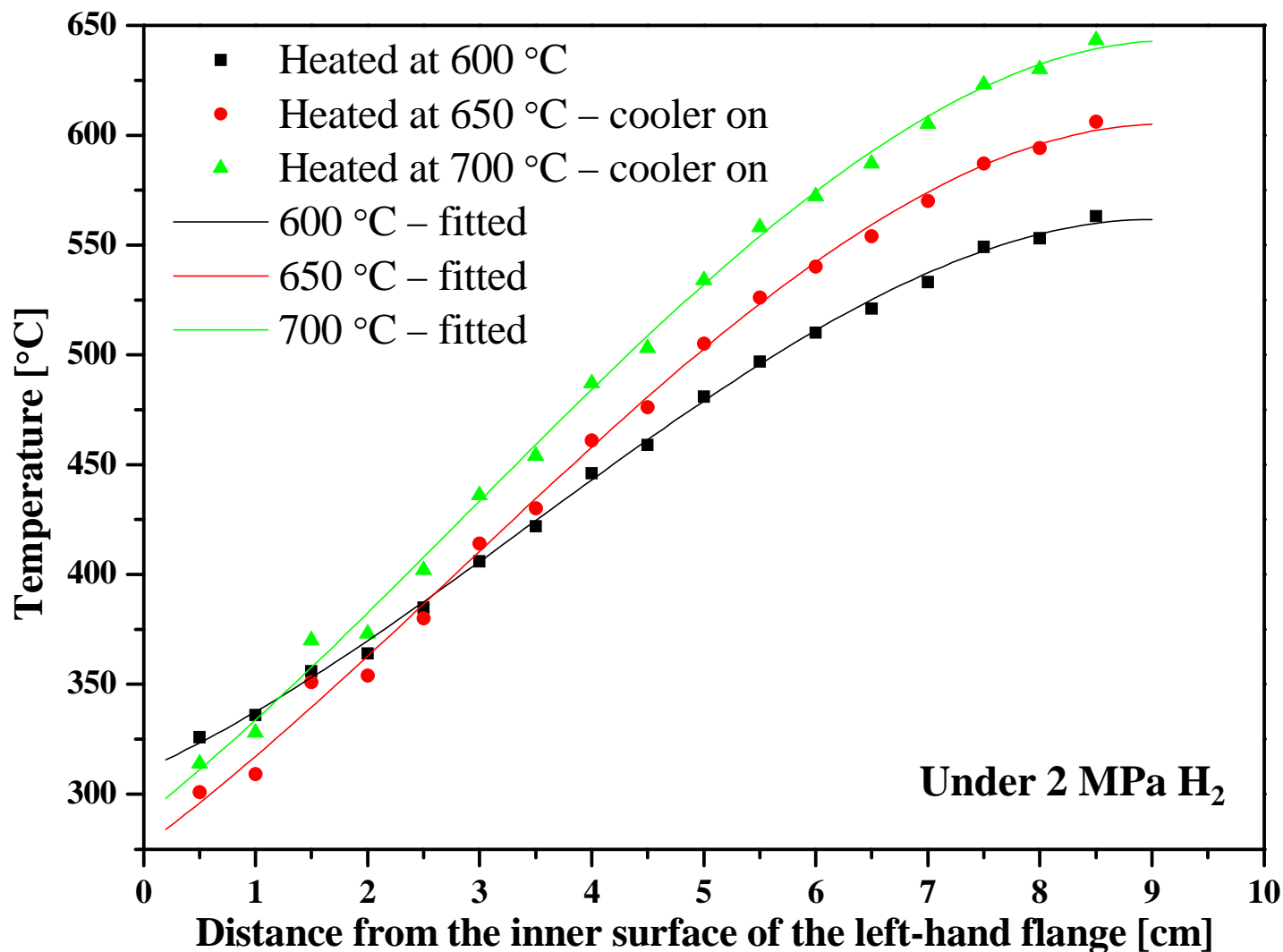
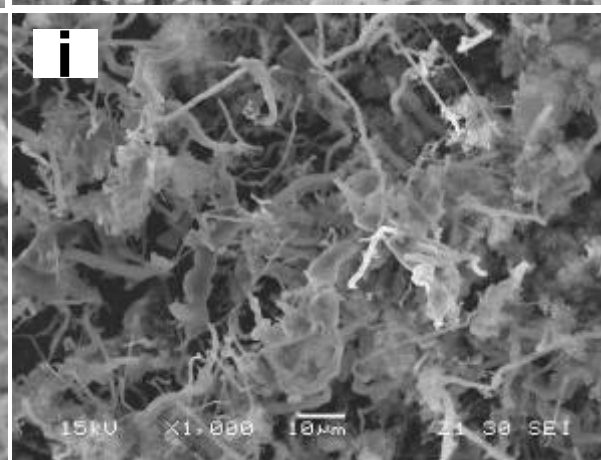
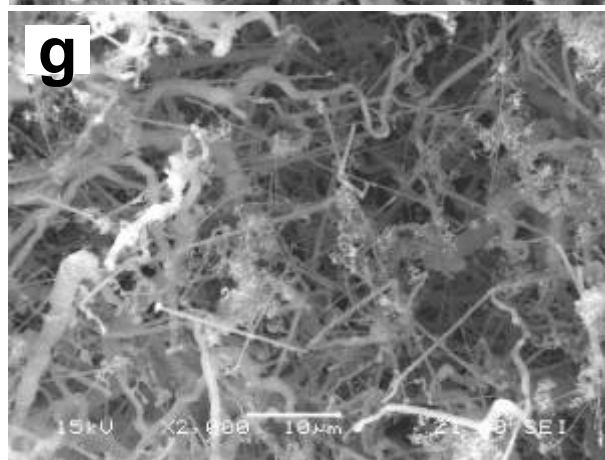
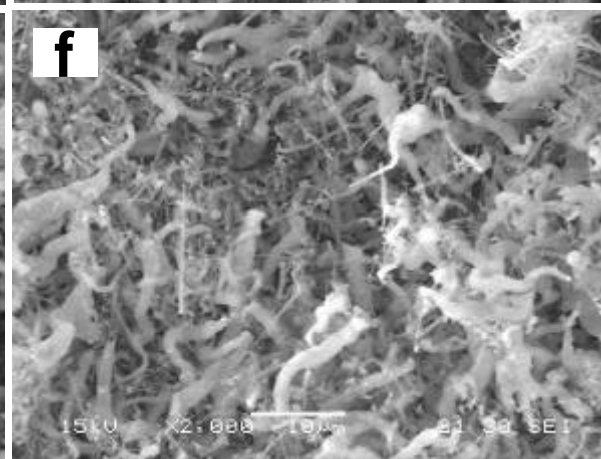
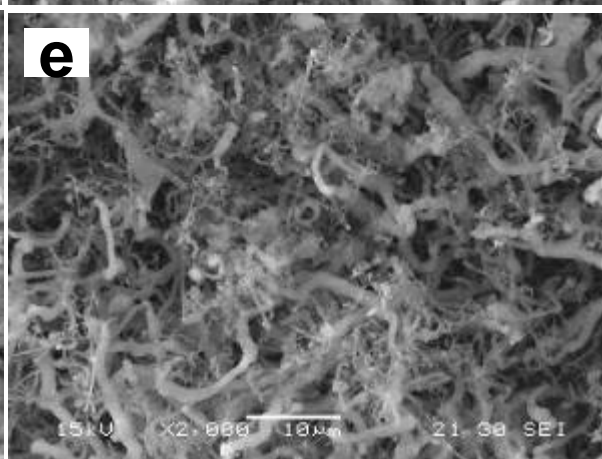
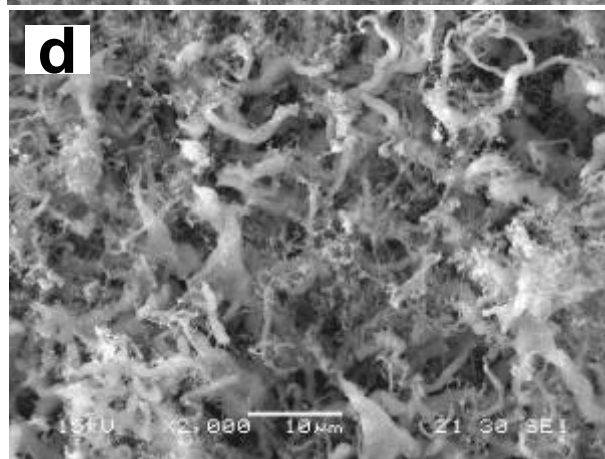
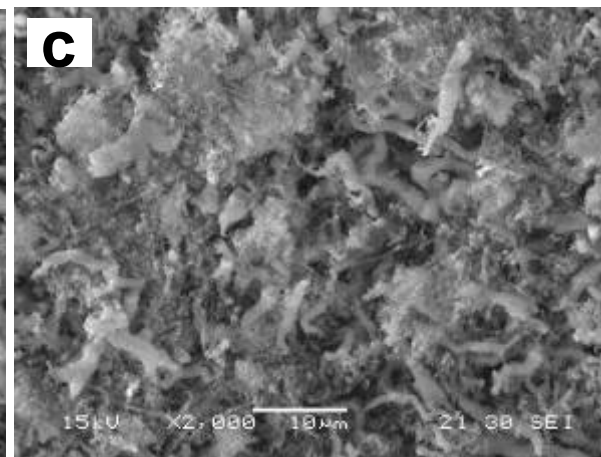
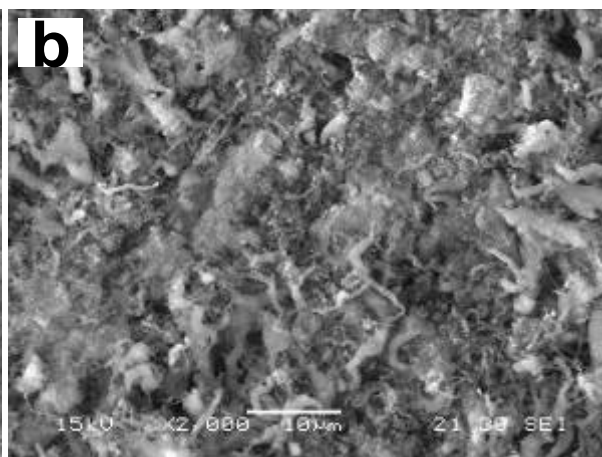
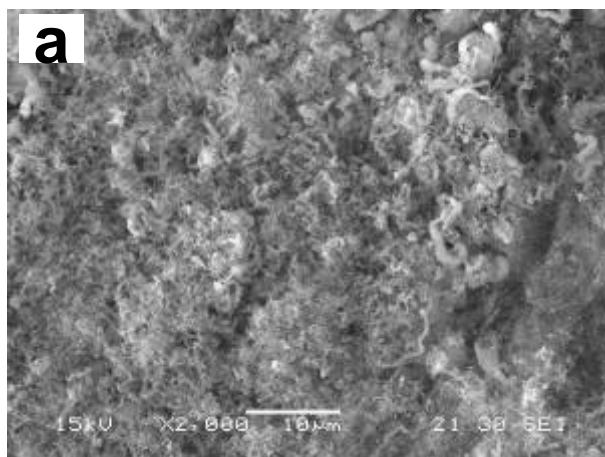


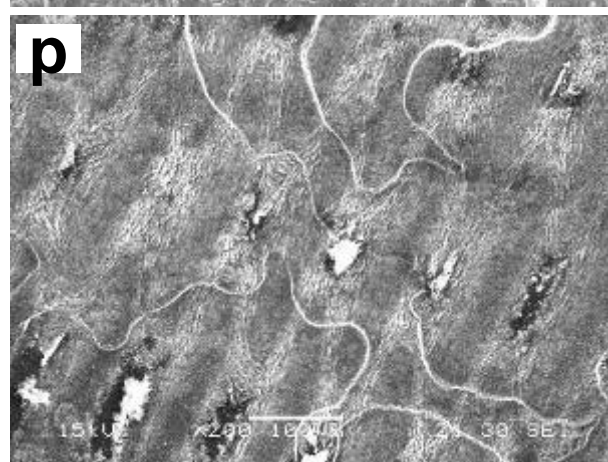
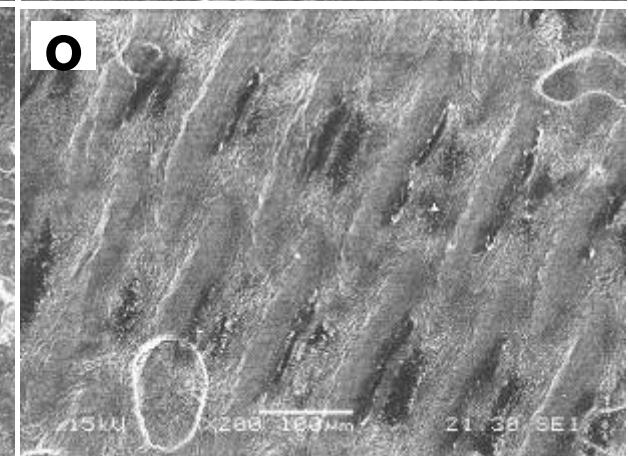
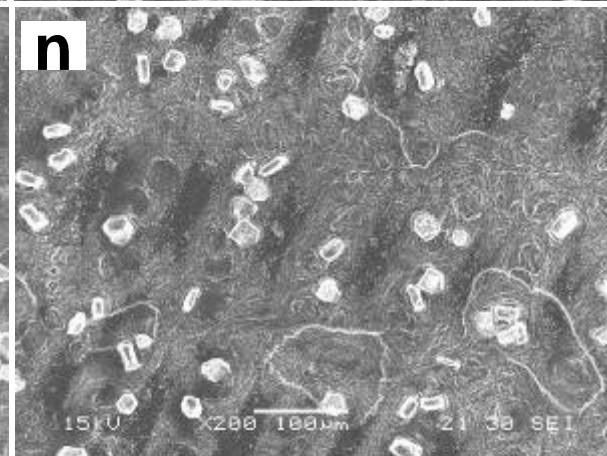
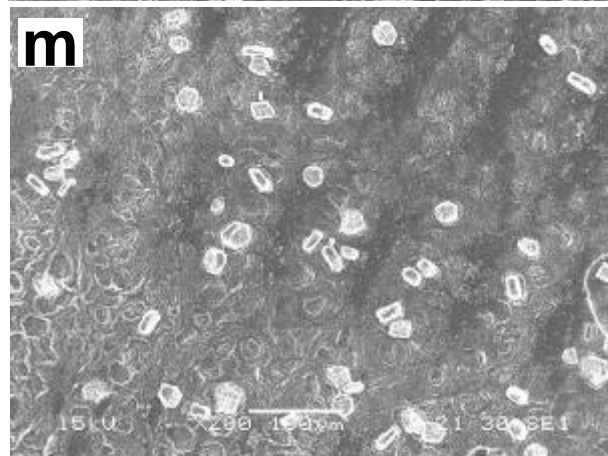
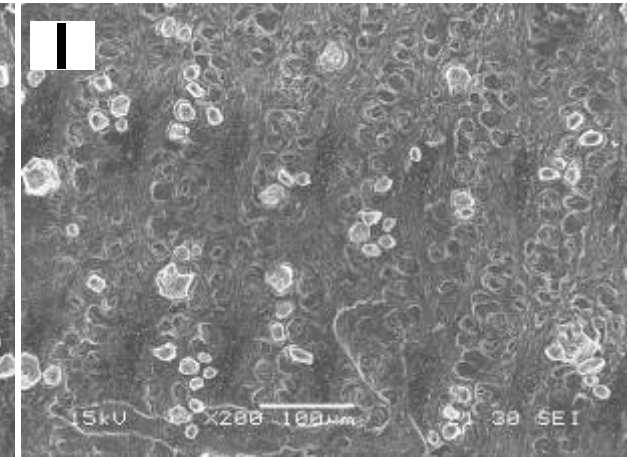
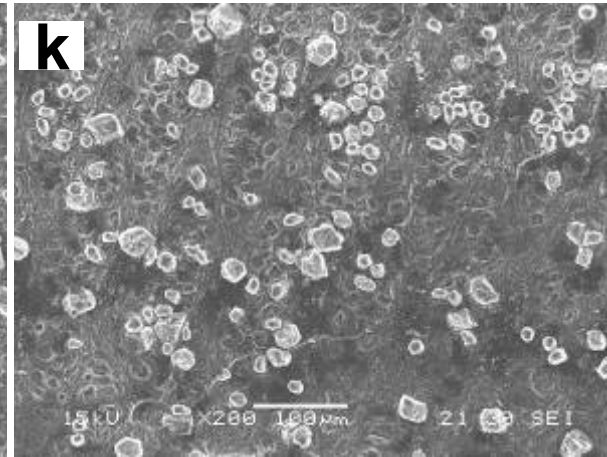
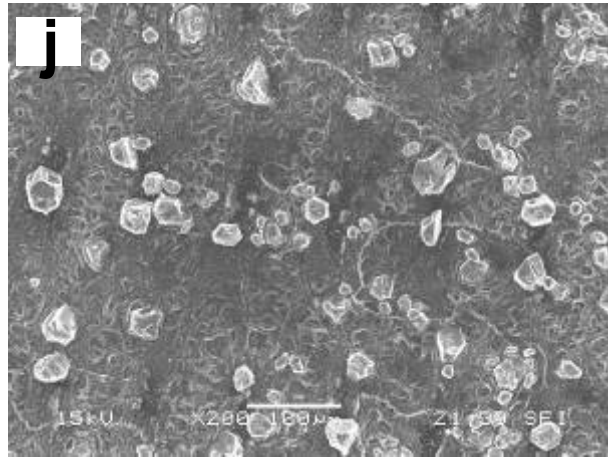
Figure S3 – (2). Temperature distribution on the mesh adhered along the tube wall under 2 MPa H₂ pressure at different evaporation temperatures. To make sure that the lowest deposition temperature is below 300 °C, a cooler jacket was set around the flange with the evaporation temperature of 650 and 700 °C.

Figure S3 – (3). 2 MPa SEM images

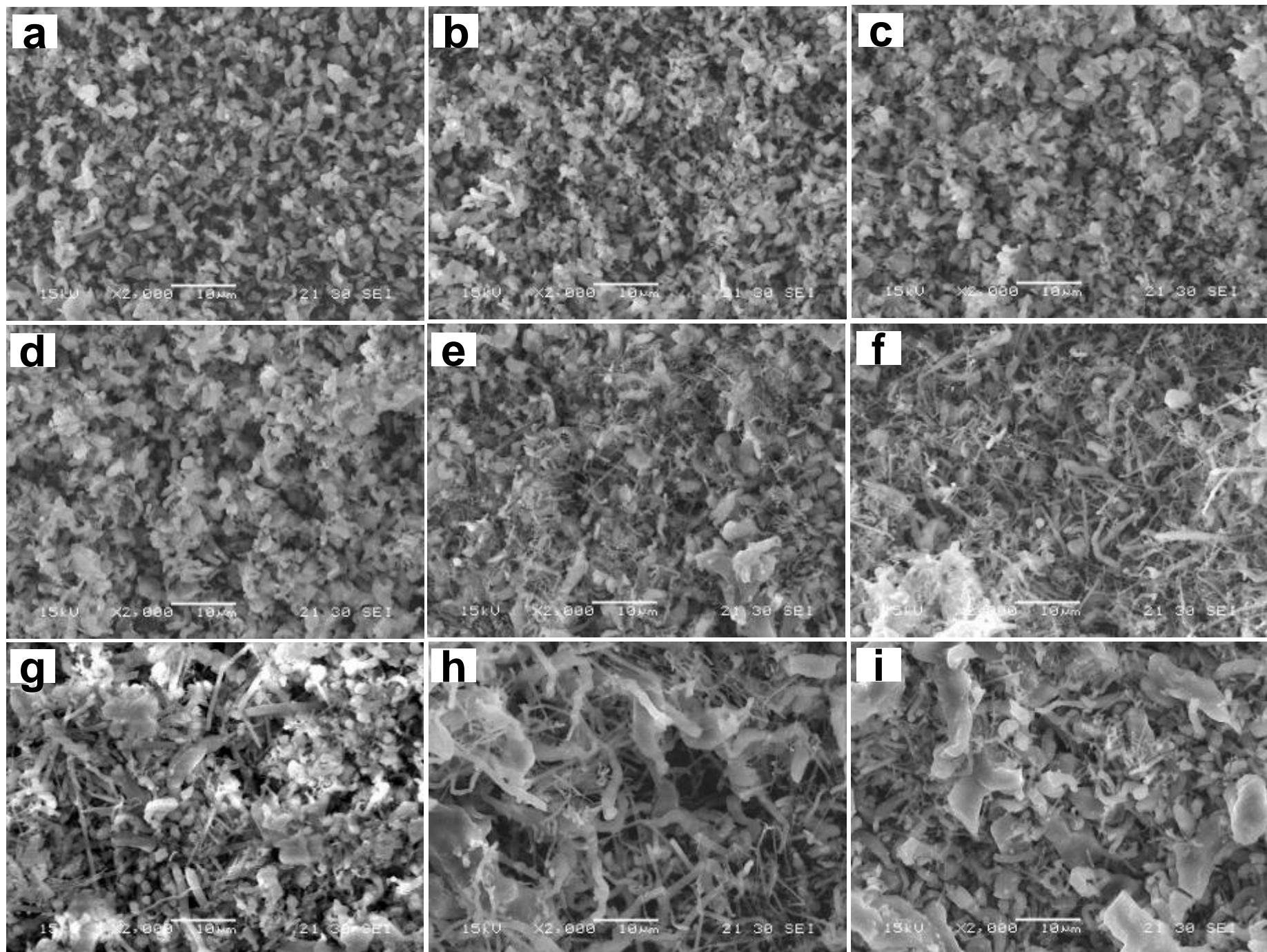
2 MPa – 600 °C



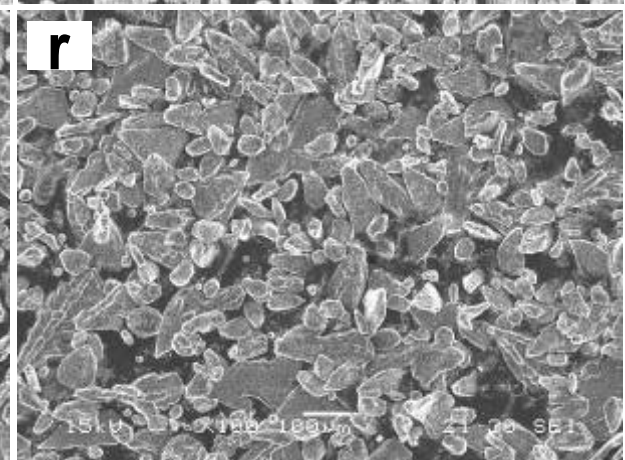
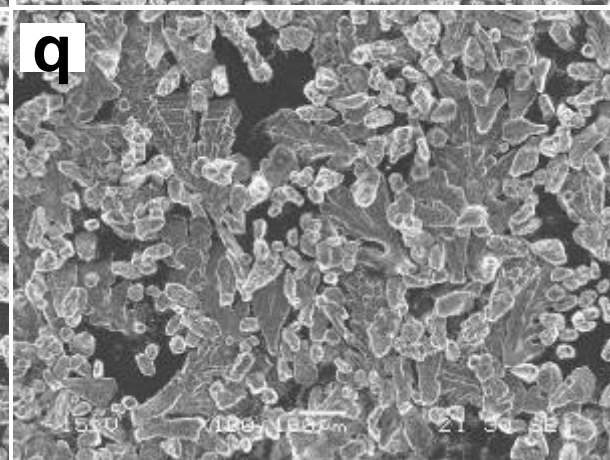
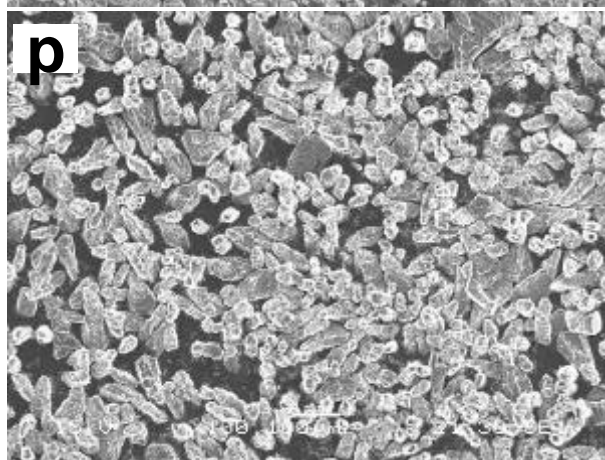
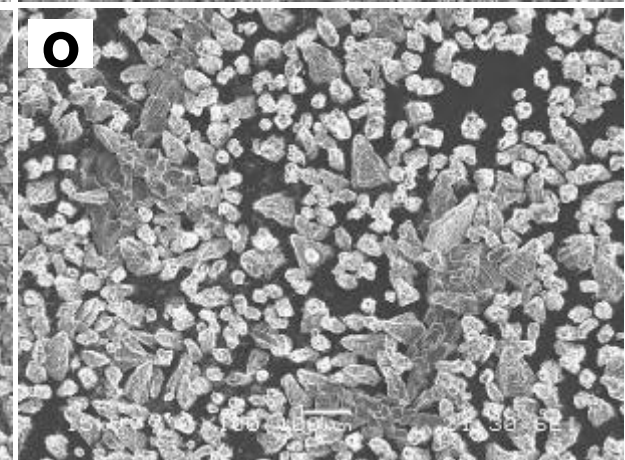
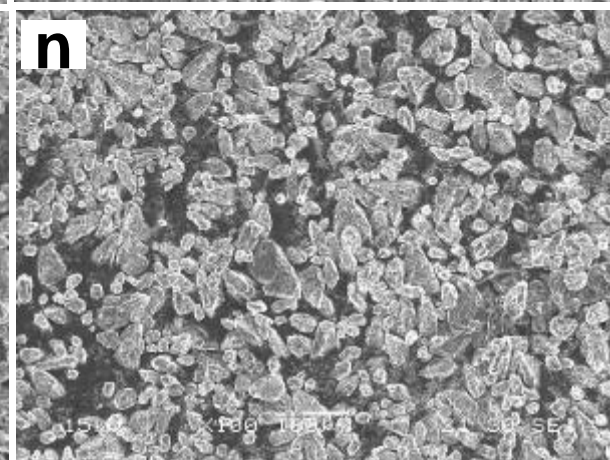
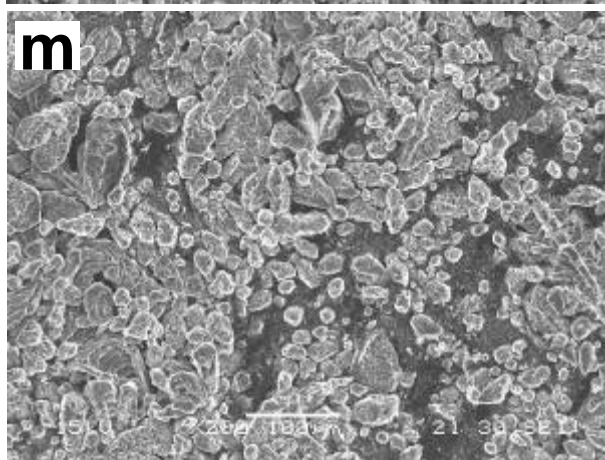
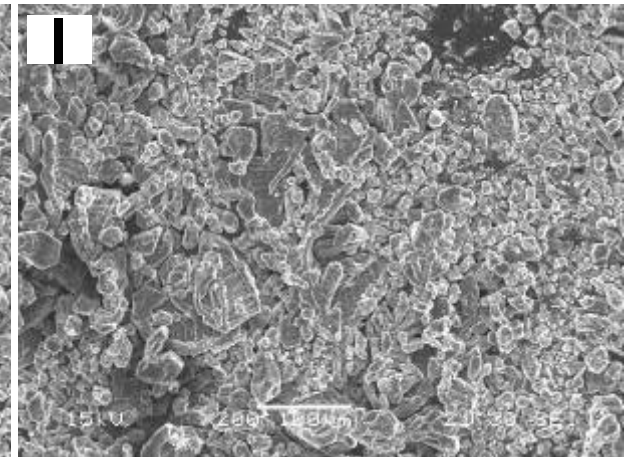
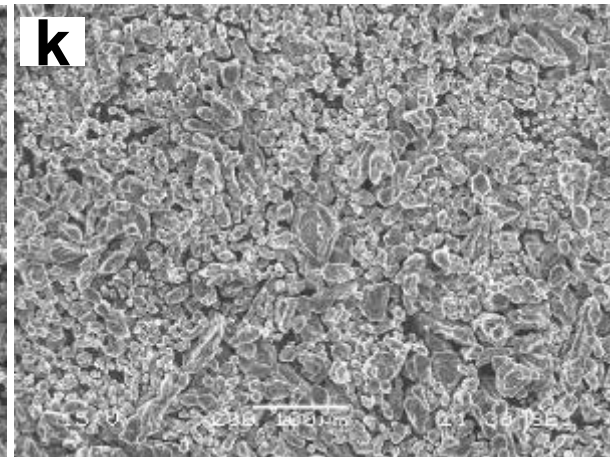
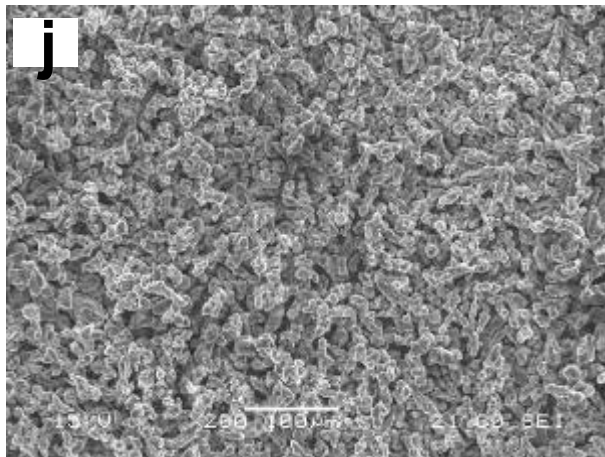
2 MPa – 600 °C



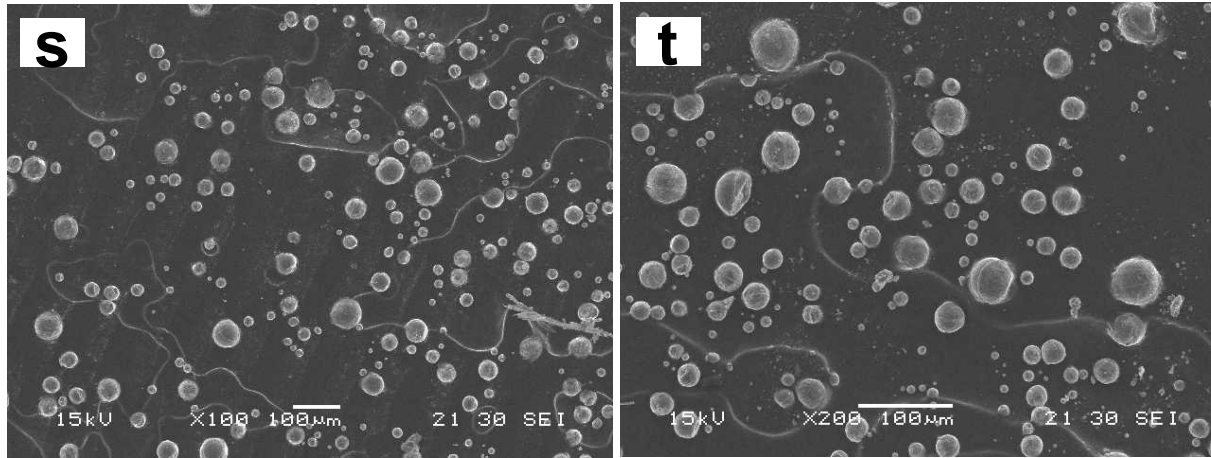
2 MPa – 650 °C



2 MPa – 650 °C

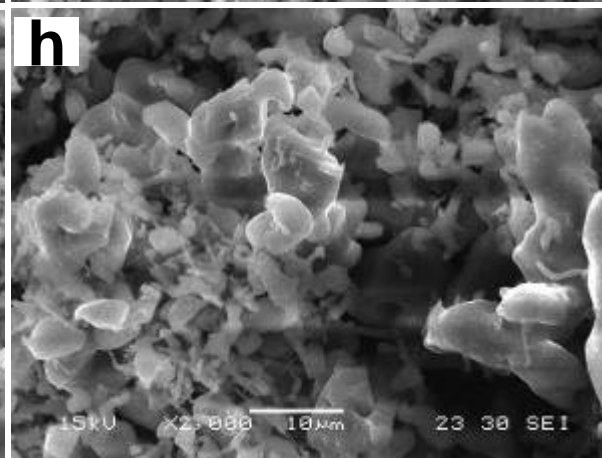
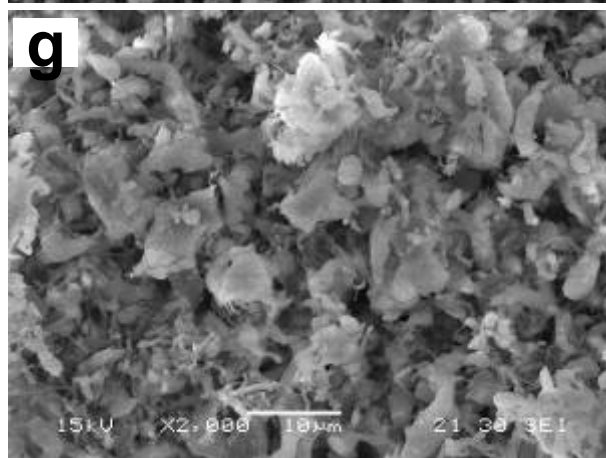
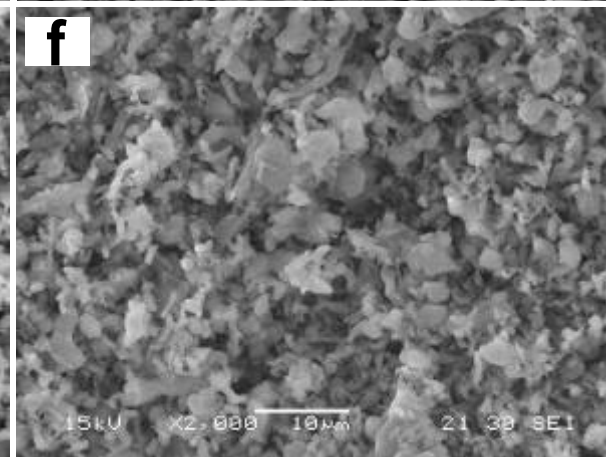
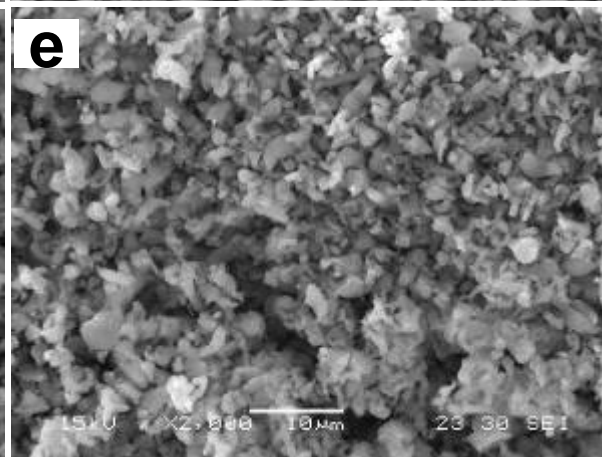
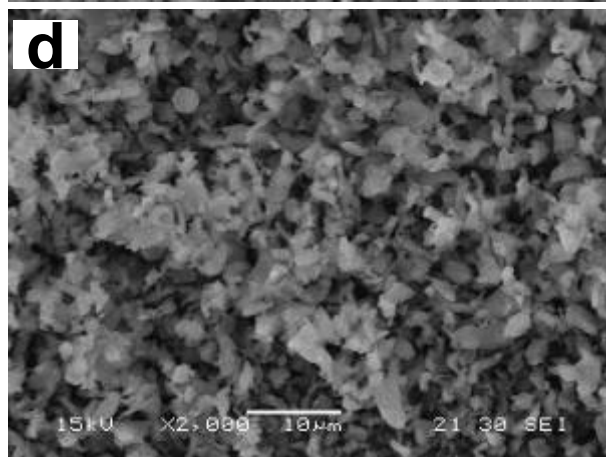
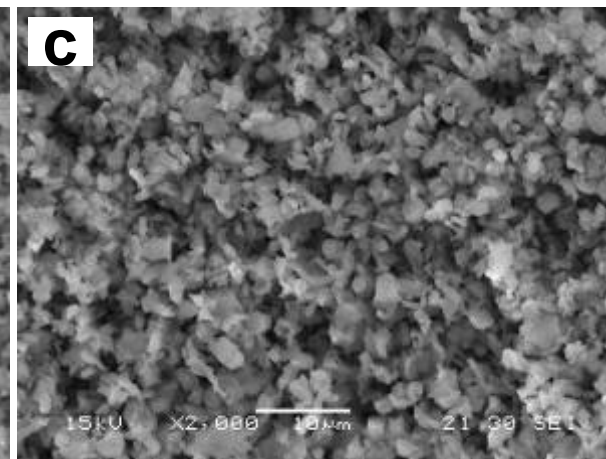
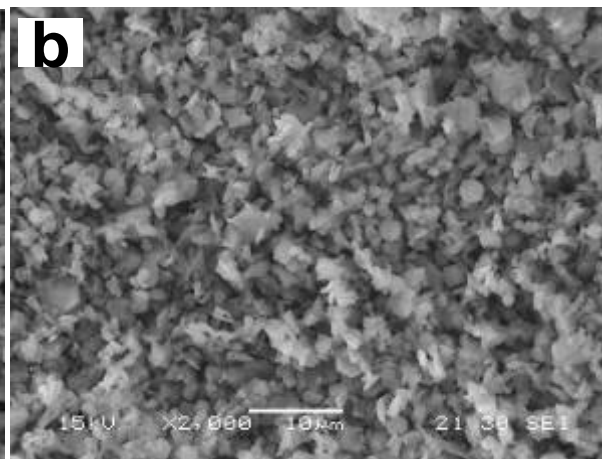
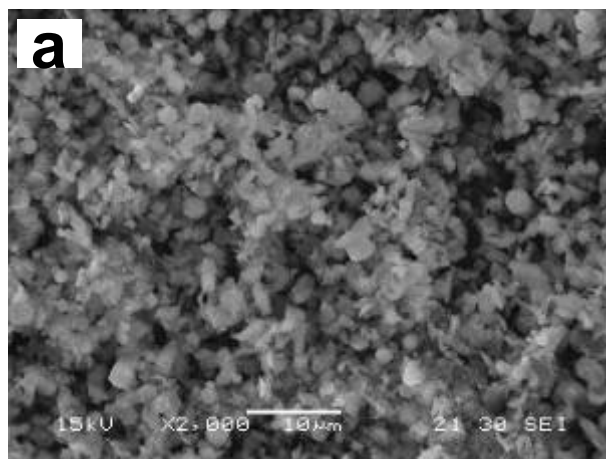


2 MPa – 650 °C



The spherical shapes can be found at a certain growth condition (heating time and evaporation temperature) at the high temperature side; with the growth time, these spheres will disappear to form hexagonal shapes or dendritic shapes.

2 MPa – 700 °C



2 MPa – 700 °C

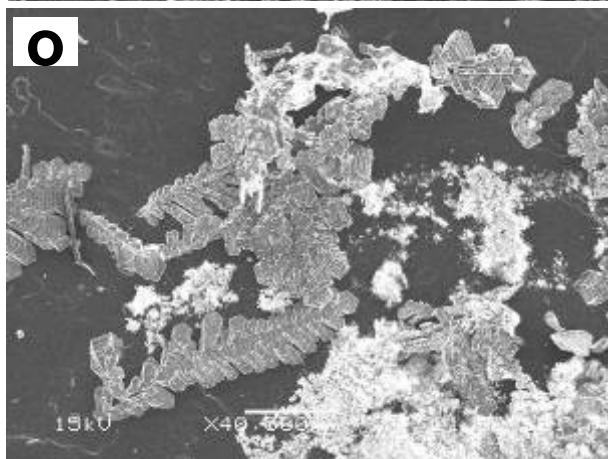
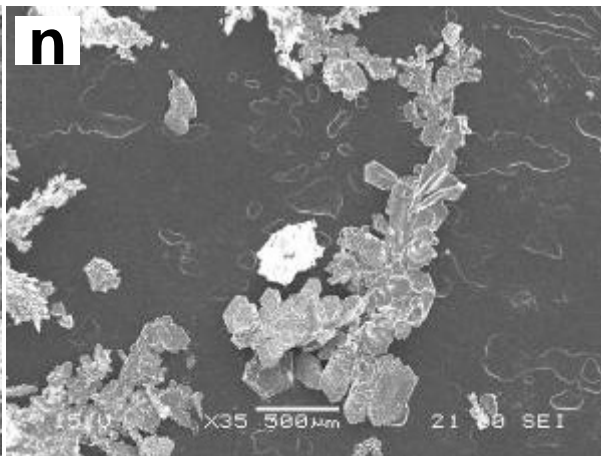
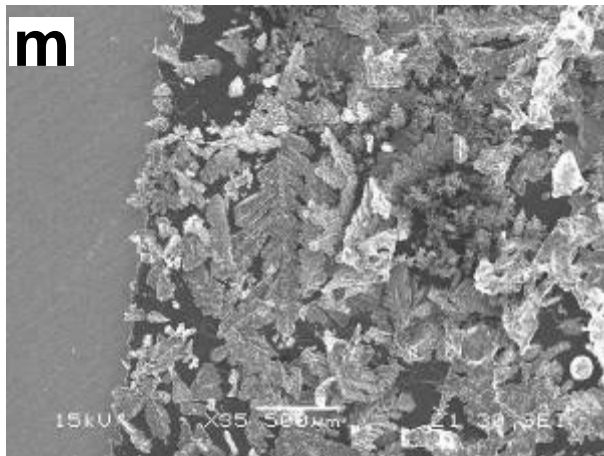
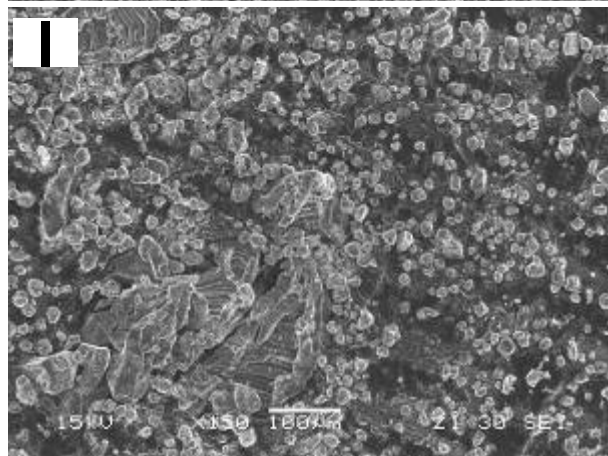
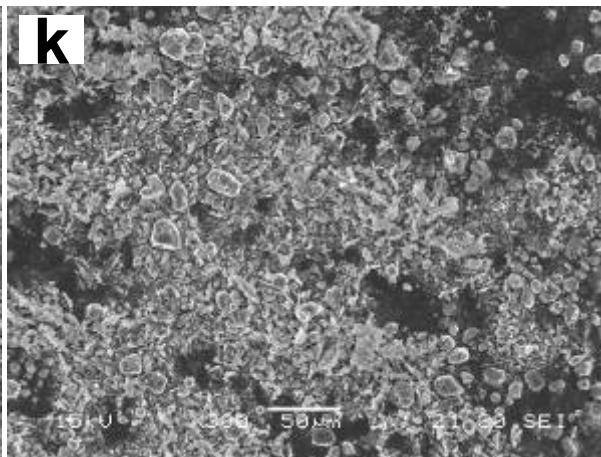
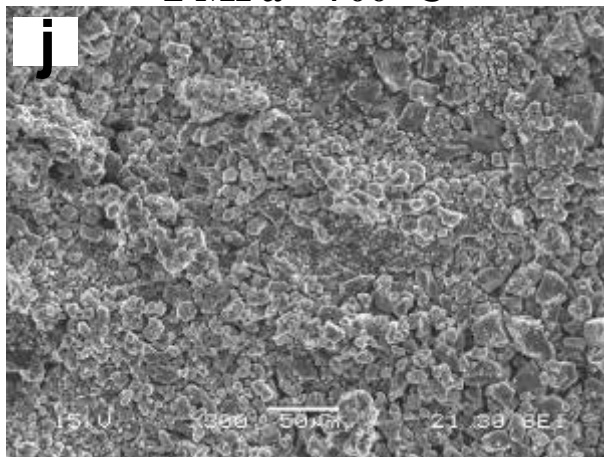
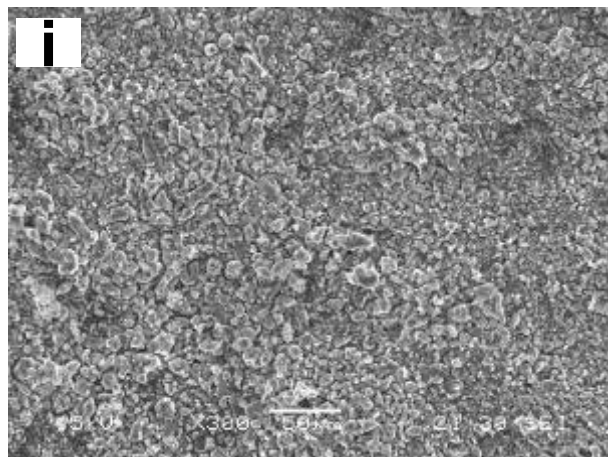
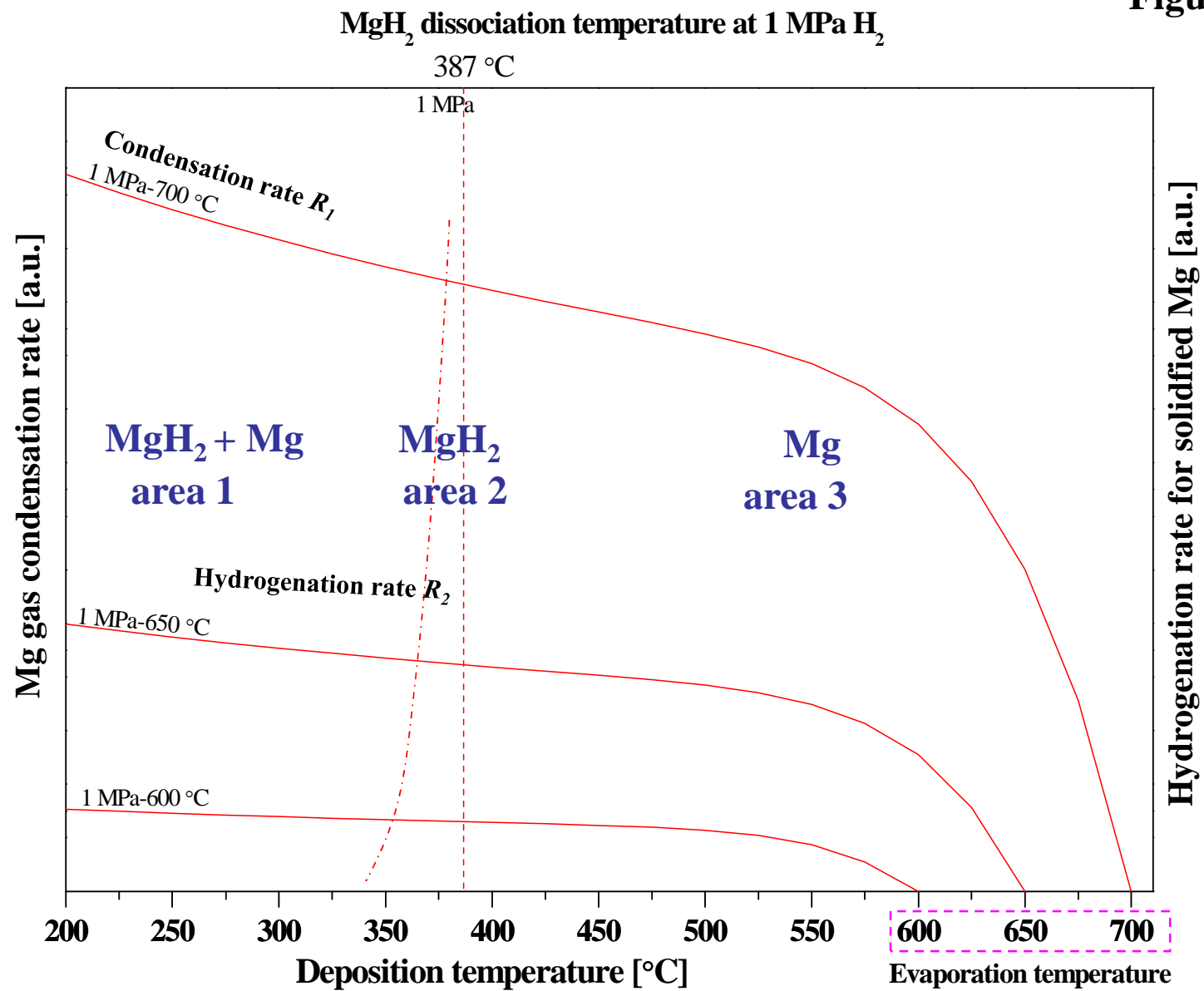


Figure S4. The calculated condensation rate for Mg gas as a function of deposition temperature under 1 and 2 MPa H₂ with evaporation temperatures of 600, 650, and 700 °C (the solid lines), respectively. The as-proposed hydrogenation rate for the solidified Mg as a function of deposition temperature under 1 and 2 MPa H₂ is plotted in the dash-dot lines; the hydrogenation rate curves were plotted based on the results of sample distribution obtained with a heating time of 4 hours.

From this figure, we can confirm that: (1) above the dissociation temperature at a certain H₂ pressure, only Mg deposits are obtained; (2) below the dissociation temperature, when $R_2 > R_1$ high-purity MgH₂ is produced, and when $R_1 > R_2$ a mixture of MgH₂ and Mg is obtained; (3) a high H₂ pressure offers a larger high-purity MgH₂ production area; and (4) the composition of the products under other growth conditions can be predicted using this figure.

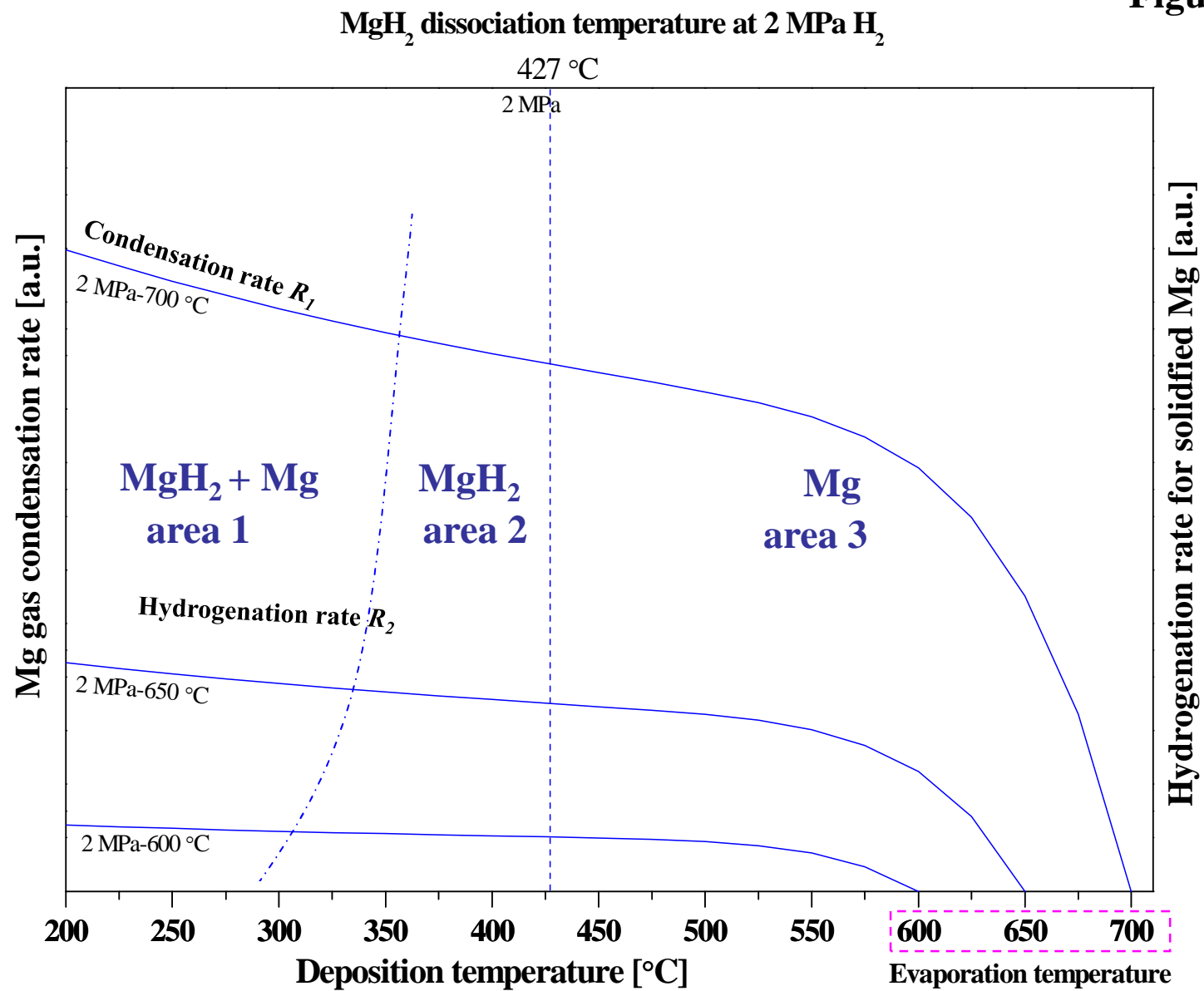
1 MPa

Figure S4



2 MPa

Figure S4



A combined one

Figure S4

