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Professor Bong-Joong Kim's joint research team identifies the spontaneous generation principle of metal nanocatalyst particles that do not coalesce at high temperatures

☐ GIST (President Kiseon Kim) Professor Bong-Joong Kim of the School of Materials Science and Engineering and KAIST Professor WooChul Jung's joint research team were the first to identify the principle behind the formation of metal catalyst particles ex-solved * when a high-temperature reducing atmosphere was formed on an oxide substrate through real-time observation in a transmission electron microscope **.

> * ex-solution: a phenomenon in which a specific metal component is separated from a specific oxide substrate or a support (mainly an oxidized substance of a perovskite structure, such as ABO 3) at a high-temperature reducing atmosphere (700 to 800° C or more in hydrogen atmosphere)
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> ** transmission electron microscope: a microscope that can magnify and view hundreds of thousands of times by letting a thin material pass through a high-voltage electron beam

- By observing particle growth at the atomic level, the researchers also succeeded in controlling the size, density, and distribution of particles that determine the characteristics of catalysts by adjusting the size and distribution of temperature and grain *.

* grain: regions having the same atomic arrangement in a crystalline material

☐ The ex-solution of the metal catalyst particles with the oxide support does not cause coarsening * even at high temperature because the catalyst particles are embedded on the surface of the support, which has been considered very important for high temperature catalytic reactions (e.g. gas sensors, fuel cells, etc.) and renewable energy (e.g., gas-sensors, etc.) as catalytic particles are embedded in the surface of the support. However, because existing studies relied on sample analysis after ex-solution, they could not understand the principles of controlling the size, density, and distribution of particles. This made it impossible to maximize the activity and durability of the catalyst.

* coarsening: in nanocatalyst particles with large chemical potential energy and small particle size, the size and density of catalyst particles change momentarily as atoms move to nanocatalyst particles with small chemical potential energy and large particle size

☐ In this study, a real-time transmission electron microscope technique with excellent atomic resolution and rapid imaging acquisition (e.g., 30 frames per second) was used to define and model growth mechanisms by understanding the kinetic mechanics of the elongation of cobalt (Co) metal elements in the $SrTi_{0.75}Co_{0.25}O_{3-\delta}$ polycrystalline substrates.

- The researchers discovered that particle size can be controlled only by temperature. In addition, all of the ex-solved metal particles were generated only at grain boundaries *, and the elution temperature was reduced to 500° C, and the grain size and distribution could be controlled to optimize the particle density and distribution. In addition, a thermodynamic model was developed to identify the rate limiting step ** of particle growth, the formation of vacancies (entangled crystal lattice positions), the enthalpy of enthalpy ***, and the activation energy **** for particle growth.

* grain boundary: area where crystals meet and form because of the high degree of free energy due to discrepancies in atomic coupling

** rate limiting step: the reaction rate is determined by the highest reaction speed due to the high energy barrier

*** enthalpy: the energy that can be drawn from a thermodynamic system, defined as the sum of the internal energy and the energy available from occupying the system volume

**** activation energy: minimum energy required for a particular chemical reaction to proceed

◦ In addition, carbon monoxide (CO) reduction reaction experiments were conducted and found that the reaction site of the catalyst formed on the oxide substrate is the boundary between the metal and the oxide substrate, and this was verified with calculations.

☐ Professor Bong-Joong Kim said, "The results of this research are the first quantitative analysis of the ex-solution of metal catalysts by using the grain phenomena. This is expected to bring about significant improvements in areas such as gas sensors and electric cars.

☐ This research was led by GIST Professor Bong-Joong Kim (corresponding author) and KAIST Professor WooChul Jung (co-corresponding author) and was supported by the Samsung Research Funding Center of Samsung Electronics. The paper was published online in the *Journal of the American Chemical Society*, a leading authority in the chemical industry, on April 2, 2019.

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