Analysis for Packing State of the Packed Bed of Hydrogen Storage Alloy Using Discrete Element Method

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Numerical analysis was performed by Discrete Element Method in consideration of expansion and contraction of particles to investigate the stress developed on the wall in the vessel of the packed bed of hydrogen storage alloy. For the packed bed composed of the spherical particles with a diameter of 2 and 7 mm, the effect of the expansion and contraction of the particles on the packing ratio and the stress developed on the wall was investigated. It was shown that smaller particles moved through the gaps between the particles by repeating expansion and contraction of particles, and the packing ratio and the stress became higher at the lower part of the packed bed. The effect of the expansion and contraction of the particles on the packing ratio and the stress developed on the wall in the vessel was also examined for the packed bed composed of the spherical, tetrahedral or cubic particles. The packing ratio in each region and the stress developed on the wall in the vessel were different depending on the shape of particles. From these results, it was shown that the shape and the movement of the particles affect the stress developed on the wall.

Key Words
Discrete Element Method, Hydrogen storage alloy, Absorption/desorption, Packing state, Stress analysis

1. Introduction

Hydrogen storage alloy can store hydrogen with high volume density by reacting with hydrogen and forming a metallic compound under the condition close to normal pressure and room temperature. Hydrogen storage alloy causes its lattice expansion when it absorbs hydrogen into its crystal lattice. When the crystal lattice non-uniformly expands in alloy particles, stress develops inside alloy particles, causing volume expansion and pulverization of alloy particles. Thus, when hydrogen is repeatedly absorbed and desorbed in the packed bed of hydrogen storage alloy, alloy particles are known to segregate in the container. Since the particle segregation would cause deformation or breakage of the container, to utilize hydrogen storage alloy safely, the stress developed in the container is of importance.

Nasako et al. measured the stress developed on the wall in the cylindrical container for the packed bed of hydrogen storage alloy with the repetitive hydrogen
absorption/desorption process. In their study, when hydrogen was repeatedly absorbed and desorbed, the stress was found to increase with an increase in the number of the hydrogen absorption/desorption cycles. In addition, Qin et al. showed stress developed on the wall at the bottom of the cylindrical container and increased with an increase in the number of hydrogen absorption/desorption cycles. They also reported that alloy particles which existed at the bottom were hard to take out because they were agglomerated, and the bottom side of the container was plastically deformed when the packing ratio was high. Further, Okumura et al. measured the packing ratio and stress developed on the wall in each region of the packed bed with repetitive hydrogen absorption/desorption and showed that the distribution of the packing ratio in each region changed due to hydrogen absorption/desorption. They also indicated the region where large stress developed was formed especially at the bottom in case of the packing ratio of about 0.6 and concluded this was caused by a transfer of pulverized alloy particles toward the bottom side. Also, Okumura et al. visualized the movement of pulverized alloy particles to the bottom side by using the X-ray CT and showed that the particle shape drastically changed due to the pulverization. The above facts suggest stress development on the wall of the container significantly relates to pulverization of alloy particles and can be caused by the change in packing ratio, that is, movement of alloy particles.

Although the above-mentioned investigations are based on experiments, the use of numerical analysis is effective to study the mechanism of stress development on the wall in the packed bed of hydrogen storage alloy. Hirosawa et al. performed stress analysis using the finite element method (FEM) assuming the packed bed of hydrogen storage alloy was a continuum and reported that stress distribution was formed when the packed bed was expanded and aspect ratio in the container affected stress development on the container. Further, Dinachandran and Mohan numerically investigated the effect of height in the packed bed of hydrogen storage alloy on stress in the tangential direction on the wall when the packed bed was expanded using the FEM and showed that the larger height in the packed bed has a greater impact on strain in the tangential direction. In contrast, since hydrogen storage alloy is powder layer and each particle expands and contracts with hydrogen absorption/desorption, the discrete element method (DEM) which can directly analyze particles as they are is expected to be a quite effective approach. Although Matsushita et al. predicted the packing state of hydrogen storage alloy using the DEM and compared it with the experimental result, there was the discrepancy between the experimental and numerical result and the introduction of the models for adhesive force and contact distance change could not reproduce the experimental result. Charlas et al. evaluated stress on the container wall due to particles’ expansion using the DEM and investigated the effect of aspect ratio in the packed bed on stress developed on the wall, indicating that stress becomes larger for larger aspect ratio in height for the diameter of the packed bed. Also, Charlas et al. treated an aggregate with several particles as a single particle and investigated the effect of particle shape on stress in the container, showing that stress on the container wall is larger with an aggregate than with a particle. However, Charlas et al. did not focus on particle movement, discussed the entire behavior of the particles in the packed bed, and did not clarify the relationship between the particles’ distribution or packing ratio and stress in the packed bed. As is mentioned above, although some numerical analyses have been performed for the packed bed of hydrogen storage alloy, the numerical method for stress on the wall in the container with hydrogen absorption/desorption has not been established yet.

In the present study, we predicted packing state and stress developed in the packed bed of hydrogen storage alloy with expansion and contraction using the DEM and investigated the effect of packing state of particles on stress in the packed bed. For the purpose of validation, the vibration test for the packed bed which consists of glass beads with different diameter was performed, transport phenomena in the packed bed were numerically analyzed using the DEM, and the experimental and numerical results were compared. Next, assuming the packed bed with hydrogen storage alloy of different spherical particles in diameter, the effect of expansion and contraction processes on packing state in the packed bed was investigated. Also, the influence of the change in packing state on stress in the packed bed was discussed. Further, simulating pulverized hydrogen storage alloy, the effect of particle shapes on stress in the packed bed was numerically studied employing particles with not only spherical but tetrahedral and cubic shapes.

2. The vibration test

Two different samples in diameter were packed in the cylinder container and moved by vibration. 150 glass beads with a diameter of 2 and 7 mm for each diameter or those with 3 and 7 mm were used as samples and packed in the acrylic cylinder container with an inner diameter of 30 mm. The container was fixed on the vibration test machine (VS-150-1, IMV) and sinusoidally oscillated in the
horizontal direction with the condition listed in Table 1. After the test, the heated agar was put in the container and the glass beads were fixed by cooling and solidifying. The agar solidified with glass beads were carefully taken out from the container. Then, the packed bed of glass beads with solidified agar was cut with an interval of 20 mm from the bottom of the container as shown in Fig. 1 and the number of glass beads for each diameter in each region were measured. To test the reproducibility, the experiment was performed ten times.

### 3. Numerical analysis

#### 3.1 Discrete Element Method

The discrete element method (DEM) was proposed by Cundall and Strack. In the DEM, contact forces such as repulsive force and the friction force which act between particles were modeled and motion of each particle on which contact force acts is traced based on the equation of motion for each particle. The motion of each particle consists of translational and rotational motion, and these equations are expressed by the following equations:

\[
\begin{align*}
\dot{x} &= \sum F_x + mg, \quad (1) \\
\dot{\omega} &= \sum T
\end{align*}
\]

Here, \( F \) is the contact force working to the focused particle, \( g \) is the gravitational acceleration, \( I \) is the inertia moment of the particle, \( m \) is particle mass, \( T \) is the torque generated by contact, and \( x \) and \( \omega \) are the location and angular velocity of the particle, respectively.

The contact force can be divided into normal and tangential components. In the DEM simulation, although solid particles are assumed rigid body that does not deform, the overlap of the particles in contact is allowed at the time of the calculation of the contact force. By multiplying this overlap and spring constant, the elastic force is calculated.

In this study, the Voigt model which has been employed in several studies was used as a contact model. The Voigt model is composed of a spring, a dashpot, and a slider. Considering the contact of the two solid particles, the normal component of the force is the following equation:

\[
F_n = -k_n \delta_n - \eta_n v_n
\]

Here, \( k_n \) and \( \eta_n \) are the spring constant and viscous damping coefficient in the normal direction, respectively. \( \delta_n \) and \( v_n \) show the displacement and relative velocity of the particle in the normal direction, respectively. The viscous damping is modeled using the dashpot assuming that the phenomenon of attenuating of energy by contact and collision between particles. Viscous damping coefficient \( \eta_n \) is given by Eq. (4) as:

\[
\eta_n = -2 \sqrt{\frac{m \kappa}{\pi \ln(e^{-1})}} \ln(e).
\]

Here, \( e \) is the restitution coefficient. When there is no slip on the surface of the solid particle, the tangential component of the contact force is expressed by the following equation:

\[
F_t = -k_t \delta_t - \eta_t v_t
\]

Here, \( k_t \) and \( \eta_t \) are the spring constant and viscous damping coefficient in the tangential direction, respectively. \( \delta_t \) and \( v_t \) are the displacement and relative velocity of the particle in the tangential direction, respectively. The viscous damping coefficient in the tangential direction was assumed that equal to that in the normal direction. On the other hand, when slip occurs, in other words, when Eq. (6) holds, the contact force in the tangential direction is given by Eq. (7):

\[
|F_t| > \mu |F_n|
\]

\[
F_t = -\mu |F_n| \frac{v_t}{|v_t|}
\]

Here, \( \mu \) is the friction coefficient.

Non-spherical particles were modeled by using an aggregate of multiple elements as one element as like the method of Favier et al. The motion of the aggregate was traced by collecting forces applied to each particle constituting the aggregate at the center of gravity of the aggregate. Furthermore, using the moment of force with respect to the center of gravity of the aggregate, the motion of the aggregate was expressed by rotating the local coordinate system \((X, Y, Z)\) with the center of gravity the aggregate as the coordinate center. The position \( x_i \) of component \( i \) of the aggregate \( k \) is expressed by the following equation:

\[
x_i = x_k + A_i X_i
\]

Here, \( x_k \) is the position of the center of gravity of the aggregate \( k \), and \( X_i \) is the position of the element \( i \) in the
local coordinate system. \( \mathbf{A} \) is a transformation matrix from the local coordinate system to the absolute coordinate system. The coordinate axes of the local coordinate system were obtained from the inertia tensor of the aggregate. The eigenvectors are the principal axis of inertia and are the coordinate axis of the orthogonal coordinate system with the center of gravity of the aggregate as the origin. The angular velocity \( \omega = [\omega_x, \omega_y, \omega_z] \) of the aggregate in the local coordinate system was obtained by solving the Euler’s equation of motion shown below.

\[
I_x \frac{d\omega_x}{dt} - (I_z - I_y) \omega_y \omega_z = N_x, \\
I_y \frac{d\omega_y}{dt} - (I_z - I_x) \omega_x \omega_z = N_y, \\
I_z \frac{d\omega_z}{dt} - (I_x - I_y) \omega_x \omega_y = N_z. 
\]  

(9)

Here, \( I_x, I_y, \) and \( I_z \) are the eigenvalues of the inertia tensor and are the main moment of inertia. \( N_x, N_y, \) and \( N_z \) are the moment of force in the local coordinate system.

### 3.3 Stress developing with expansion and contraction of hydrogen storage alloy

To discuss the packing state of the packed bed and the stress developed on the wall with expansion and contraction of hydrogen storage alloy, for the packed bed composed of particles of different diameters, each particle was expanded and contracted, and the packing ratio of the packed bed and the stress developed on the wall in the container were computed. 150 particles with a diameter of 2 and 7 mm for each diameter were packed in the cylinder container with an inner diameter of 30 mm. Then, referring to the lattice constant of \( \text{LaNi}_5 \) and \( \text{LaNi}_5\text{H}_6 \), the particle diameter was increased up to the maximal volume expansion rate of 0.273 with the expansion rate of 0.273 \( \text{s}^{-1} \) at which the packed bed expanded stably and decreased to the original diameter with the same rate. The above expansion/contraction process was defined as one cycle, and the stress on the wall and the packing ratio in the packed bed at each cycle were evaluated by repeating the cycle ten times. Also, to analyze the local stress and packing ratio in the packed bed, the packed bed was divided into four parts in the axial direction with an interval of 20 mm from the bottom side of the container, which were named as Region 1, 2, 3, and 4, respectively. The estimation method of the stress developed on the wall is described in the appendix, and the packing ratio of each region was calculated by dividing the total volume of the particles existing in the region by the volume of the region. Assuming expansion and contraction of hydrogen storage alloy of \( \text{LaNi}_5 \), the spring, restitution and friction coefficients were prescribed as in Table 3, and the time increment was set to \( 1.0 \times 10^5 \) s. The same values of the spring constant and the time increment for the vibration test was used to reduce computational time. Since the restitution and friction coefficients are not available for \( \text{LaNi}_5 \), the measured values for the similar metal of Cu and Ni were used \( ^{19} \). The initial arrangement of the particles was the same as in subsection 3.2.

Next, since the packed bed of hydrogen storage alloy consists of complex particles in shape, the effect of shapes in non-spherical particles on stress developed on the wall was investigated. Non-spherical particles were expressed regarding an aggregate as a single particle, the single spherical, tetrahedral and cubic particles shown in Fig. 2.

### Table 2 Numerical parameters of glass beads

| Parameter          | Value          |
|--------------------|----------------|
| Element density    | 2500 kg/m³     |
| Spring constant    | \( 1.0 \times 10^4 \) N/m |
| Restitution coefficient | 0.95          |
| Friction coefficient | 0.7            |

### Table 3 Numerical parameters of hydrogen storage alloy

| Parameter          | Value          |
|--------------------|----------------|
| Element density    | 8300 kg/m³     |
| Spring constant    | \( 1.0 \times 10^4 \) N/m |
| Restitution coefficient | 0.3            |
| Friction coefficient | 0.6            |
were employed. The single spherical particle has only one element, the tetrahedral one consists of five elements with the arrangement of one element on gravity center and the others on vertex, and the cubic one has 27 elements with a diameter of 2 mm arranged to inscribe cube with a side of 4 mm. Each particle was set to have a volume of 64 mm$^3$, and the diameters of the elements forming the spherical and tetrahedral particles were 4.96 and 2.9 mm, respectively. 100 non-spherical particles were packed in the cylinder container with an inner diameter of 20 mm and the same analysis as the one with two kinds of particles different in diameter was conducted assuming hydrogen absorption/desorption. Note that the number of expansion and contraction cycles was set to three at which the packing ratio and stress developed did not change anymore.

4. Results and discussion

4.1 Validation of the vibration test

Fig. 3 (a) shows the measured and predicted number of smaller particles in each region in the packed bed of the glass beads with diameter of 2 mm and 7 mm after the vibration test and Fig. 3 (b) displays the predicted particle distribution in the packed bed of the glass beads before and after the vibration test, respectively. Since the small particles moved to the bottom side of the packed bed through the gap between the large particles by the vibration, the number of the particles with a diameter of 2 mm was the smallest in Region 4 which was located on the top side and the number increased toward to the bottom side. Also, the large particles slightly move by the vibration and the packing state converges to the closest packing and the gap between the large particles becomes smaller. Thus, all the small particles could not move to the bottom side and the small particles existed not only in Region 1. Focusing on the numerical results, they are in good agreement with experimental ones in each region of the packed bed after the vibration test. Further, the numerical analysis successfully predicts that while the particles with a diameter of 2 mm move from the top to the bottom side of the packed bed by the vibration, not all the particles do not. From the above results, we successfully demonstrated that the numerical analysis with the discrete element method could reproduce the movement of the small particles to the bottom side through the gap between the large particles in the packed bed which consisted of the different particles in diameter. Fig. 4 compares the experimental and the numerical results in a similar test with the glass beads with a diameter of 3 and 7 mm. Focusing on Region 1–3, the numbers of the particles with a diameter of 3 mm are almost the same values in the experiment and simulation. This is because the gap is relatively small in the packed bed with the glass beads of 3 and 7 mm in diameter than in those in 2 and 7 mm, the small particles cannot move to the bottom side through the gap and particles’ positions change little from the initial ones. As the numerical results agree with the experimental ones, the numerical analysis has a capability to describe the phenomenon in the packed bed with the glass beads with a diameter of 3 and 7 mm. Consequently, the numerical analysis with the discrete
4.2 Stress developing in the packed bed of hydrogen storage alloy with absorption/desorption process

To investigate the packing state in the packed bed of hydrogen storage alloy with the absorption/desorption process, Fig. 5 shows the averaged packing ratio in each region when the particles expanded at each cycle. The packing ratio becomes about 0.6 with an increase in the number of cycles. Since the previous research indicated the packing ratio was approximately 0.6 for the larger number of cycles, the numerical solution qualitatively reproduced the previous experiment. Focusing on Region 1, the packing ratio increased with an increase in the number of cycles and became constant for the larger number of cycles. This is because the particles move to fill the void space which existed at the initial state and then become unlikely to move much after space is filled to a certain degree. In region 2–4, the packing ratio also increased for the larger number of cycles and the reason would be the same for Region 1. Focusing on the number of cycles of 2, the packing ratio is found to become higher in Region 2 than in the others. The present packed bed consists of the particles with a diameter of 2 and 7 mm and the result would be caused by the movement of the particles with a diameter of 2 mm. As is shown in Fig. 3 (b), the 2 mm-particles move to down through the space between the 7 mm-particles and the similar behavior would be shown.

To investigate stress developed on the wall in the vessel due to the expansion of hydrogen storage alloy, Fig. 6 indicates the averaged stress developed on the wall in each region when the particles expanded at each cycle. In Region 1, the stress developed on the wall decreased for the number of cycles of 1–4. This would be because particles...
were rearranged to relax large stress caused by unevenness in the initial particle packing state. After the number of cycles of 4, the stress developed on the wall increased with an increase in the number of cycles. In Region 2–4, the stress developed on the wall in the vessel increased. This is because packing ratio increased with an increase in the number of cycles as shown in Fig. 5. Further, it is thought that the larger stress developed in the region with a higher packing ratio because the larger stress was shown in the lower part of the bed where the packing ratio is higher. However, although the packing ratio in Region 2 is almost the same as that in Region 1, stress on the wall in Region 2 is much smaller than that in Region 1. Therefore, stress on the wall would develop easily in the lower part of the packed bed. This is because the particles in the lower part of the packed bed are likely to be compressed by the packed bed weight themselves.

To evaluate the relationship between the packing state in the packed bed of hydrogen storage alloy and stress developed on the wall in the vessel, Fig. 7 shows the relationship between the packing ratio in each region during the swelling of particles and stress developed on the wall in the corresponding region. The stress developed on the wall increased with an increase in the packing ratio and it drastically increased when the packing ratio exceeded 0.55. Okumura reported that the packing ratio was higher in the lower region of the packed bed of hydrogen storage alloy and stress of over 20 MPa developed when the packing ratio showed the value of over 0.6. The numerical solution also predicted the higher packing ratio in the lower region of the packed bed and a drastic increase in stress developed on the wall of the vessel over a certain value of the packing ratio although the stress value was small due to the small spring constant. Thus, the numerical analysis can express the change in packing state and phenomenon of stress development in the packed bed of hydrogen storage alloy with hydrogen absorption/desorption.

Next, the effect of the shape of non-spherical particles on the packing state in the packed bed of hydrogen storage alloy with expansion and contraction was investigated. Fig. 8 indicates the averaged packing ratio in each region at each cycle for the spherical, tetrahedral, and cubic particles. For the spherical particles, the packing ratio slightly decreased with an increase in the number of cycles in Region 1. This would be caused by the rearrangement of the particles to relax the local stress. On the other hand, since the particles moved with filling void space in the packed bed in Region 2–4, the packing ratio increased with an increase in the number of cycles. This is the same behavior as in the above analysis. When the particles of hydrogen storage alloy are

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*Fig. 7 Relationship between stress and packing ratio in spherical particles

*Fig. 8 Averaged packing ratio in each region during swelling of particles: (a) spherical particles, (b) tetrahedron-shape particles, and (c) cubic-shape particles*
the tetrahedral and cubic one, as is the same with the spherical particles, the particles moved with filling the void space and the packing ratio increased with an increase in the number of cycles. However, the packing ratio in Region 1 also increased with the tetrahedral or cubic particles unlike with the spherical ones. This is because the friction force of the non-spherical particles for movement is larger than that of the spherical particles. In other words, even when large stress was generated locally in the packed bed, the large movement of the non-spherical particles does not occur to relax the stress. Also, the packing ratio in the case of the tetrahedral particles is lower in all regions than that of the spherical ones since the tetrahedral particles with complex shapes are unlikely to penetrate void space between particles. On the other hand, the packing ratio is higher with the cubic particles than with the spherical ones. This is because the cubic particles were packed with forming a layer. Comparing the case of the cubic particles with that of tetrahedral ones, the packing ratio drastically increased in Region 2. It is considered that this is due to the rotation of the cubic particles so that the packed bed becomes dense and stable.

The stress on the wall in the vessel of the packed bed of hydrogen storage alloy with expansion and contraction of the non-spherical particles was also investigated. Fig. 9 shows the averaged stress at each cycle in each region, which was caused on the wall in the vessel due to particle expansion. With the spherical particles, the stress developed on the wall decreased from cycle 1 to 2 in Region 1. This would be because the particles were slippery in shape compared with the others and rearranged to relax large stress caused by initial unevenness in the packing state. In Region 2–4, although the large change was not found, the entire tendency was decreased. This result would be caused by the movement of particles for a stable arrangement to fill void space. Also, as is the same with the result in Fig. 6, the stress developed on the wall in the lower part of the packed bed became higher because the packed bed was compressed by the packed bed weight itself. With the tetrahedral particles, the stress on the wall in Region 1 decreased as with the case of the spherical particles and the one in the other regions slightly decreased. The stress in the packed bed with the tetrahedral particles was smaller than that with the spherical ones in this study although Charlas et al. 13 showed the stress with the tetrahedral particles in the packed bed is larger when the particles were packed, expanded and contracted. Okumura et al. 7, 21 experimentally indicated the stress became larger in the region with higher packing ratio, and the stress with the tetrahedral particles is thought to be smaller than that with the spherical ones because the packing ratio with the tetrahedral particles is lower than that with the spherical ones. On the other hand, although the packing ratio with the cubic particles are high in all the regions, the stress developed on the wall in the vessel with the cubic particles is smaller than that with the spherical ones. Since the cubic particles are packed with forming the layer and the void space in the height direction is small whereas that in the radial direction is large in the cylindrical container, the stress on the wall in the vessel with the cubic particles is thought to be smaller than that with the other ones.

To evaluate the relationship between the packing ratio and the stress in the packed bed, the packing ratio in each region and the stress on the wall in the corresponding region in the expansion process at each cycle shown in

![Averaged radial stress in each region during swelling of particles: (a) spherical particles, (b) tetrahedron-shape particles, and (c) cubic-shape particles](image-url)
Fig. 10 is discussed. With the spherical particles, the stress on the wall is the highest compared to that with the non-spherical ones and it significantly varies. This is because the spherical particles are likely to be packed more densely in the radial direction, and the large stress is thought to be locally derived. Next, with the tetrahedral particles, the variance in the packing ratio is larger than that with the spherical ones. This suggests not only the position but also the direction of the particles would affect the packed bed structure since the tetrahedral particles are directional. In addition, since the tetrahedral particles could form the packed bed with low packing ratio depending on their direction, the stress and its variance in the packed bed are low and small compared to that with the spherical ones. With the cubic particles, the packing ratio distributes as with the tetrahedral particles because the packing ratio varies according to their direction. However, the stress on the wall with the cubic particles is small and its variance is also small. As is described above, this would be void space is large in the radial direction through the particles are packed densely in the height direction. From the above, although the stress is thought to be high in the region where the packing ratio is high, and it drastically increased over the packing ratio of 0.55, showing a reasonable agreement with the previous experiment. This suggests the packing ratio correlates the stress developed in each region when the particles are assumed to be spherical. Moreover, when the same particles in size in the packed bed with the tetrahedral and cubic particles as non-spherical particles in addition to spherical particles were expanded and contracted, the distribution of the packing ratio and stress developed in the packed bed were different depending on their shape. Although the packing ratio with the spherical particles is lower than that with the cubic particles, its stress was the largest, suggesting that the particle mobility significantly affects the stress developed on the wall.

5. Conclusion

This study performed the numerical analysis for the packed bed of hydrogen storage alloy using the discrete element method and predicted the packing state of the particles and the stress developed in the packed bed. Since some particles move to the bottom side in the packed bed depending on their size when they expand and contract, the model problem in which the glass beads with a different diameter in the packed bed were vibrated was numerically analyzed, and the numerical solution was compared with the experiment and validated. Because the distribution of the smaller particles in the packed bed agreed in the experiment and simulation, it was demonstrated that the present model could describe the phenomena that the particle moved to the bottom side in the packed bed when the particle was smaller than the void space between particles. Further, focusing on the change in the packing state in the packed bed with expansion and contraction of hydrogen storage alloy with different diameter, the packing ratio became higher in the lower part in the vessel because of movement of the particles with expansion and contraction. Also, the stress developed in the packed bed was high in the region where the packing ratio was high, and it drastically increased over the packing ratio of 0.55, showing a reasonable agreement with the previous experiment. This suggests the packing ratio correlates the stress developed in each region when the particles are assumed to be spherical. Moreover, when the same particles in size in the packed bed with the tetrahedral and cubic particles as non-spherical particles in addition to spherical particles were expanded and contracted, the distribution of the packing ratio and stress developed in the packed bed were different depending on their shape. Although the packing ratio with the spherical particles is lower than that with the cubic particles, its stress was the largest, suggesting that the particle mobility significantly affects the stress developed on the wall.

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Appendix

Stress developed on the wall due to the expansion of hydrogen storage alloy was estimated in this study. Stress on the wall \( \sigma \) was calculated by following equation:

\[
\sigma = \frac{\Sigma F_w}{S},
\]

(A1)

Here, \( F_w \) shows the contact force working to the element which represented a wall, and \( S \) is the area of the wall in the cylinder container. To validate the estimation method of stress on the wall, the stress developed on the bottom of the container due to their own weight was calculated and compared with the theoretical value. In this validation, 500 particles with a diameter of 2 mm were used and put into the cylinder container with an inner diameter of 20 mm. Assuming expansion and contraction of hydrogen storage alloy of LaNi5, the spring, restitution and friction coefficients were prescribed as in Table 3.

Fig. A1 compares the theoretical and numerical solutions of stress developed on the bottom of the vessel. Since 500 particles are packed in the vessel, the theoretical stress developed on the bottom of the vessel is a constant value of 542 Pa. The numerical solution shows the value close to the theoretical one. Hereby, the reason for the oscillation in the numerical solution is that the particles slightly move in the vessel. This is because the contact force becomes larger when the particle moving continuously due to the gravity force overlaps the bottom of the vessel and then the contact force becomes smaller when the particle jumped from the bottom. From the above, we successfully demonstrated the stress developed on the bottom was reasonably estimated.

Nomenclatures

- \( A \) = Transformation matrix
- \( e \) = Restitution coefficient [–]
- \( F \) = Contact force [N]
- \( F_w \) = Contact force working to the element which represented wall [N]
- \( g \) = Gravitational acceleration [m/s²]
- \( I \) = Inertia moment [kg m²]
- \( k \) = Spring constant [N/m]
- \( m \) = Particle mass [kg]
- \( N \) = Moment of force in a local coordinate system [N m]
- \( S \) = Aria of the wall in the cylinder container [m²]
- \( T \) = Torque [N m]
- \( t \) = Time [s]
- \( v \) = Velocity [m/s]
- \( X \) = Particle location in a local coordinate system [m]
- \( x \) = Particle location [m]
- \( \delta \) = Displacement [m]
- \( \eta \) = Viscous damping coefficient [kg/s]
\( \mu \) = Friction coefficient
\( \sigma \) = Stress
\( \omega \) = Particle angular velocity

Subscripts

- \( i \) = Element \( i \)
- \( k \) = Aggregate \( k \)
- \( n \) = Normal component
- \( t \) = Tangential component
- \( X \) = x-component in a local coordinate system
- \( Y \) = y-component in a local coordinate system
- \( Z \) = z-component in a local coordinate system