

Research Article

Calculation Method of Specific Surface Area of Foam Metal Based on an Ideal Tetradecahedron Model for Lithium Ion Battery

Jian Chen,¹ Xiao Zhang,¹ Cong Li ,^{1,2} Xinyuan Zhang,¹ Yanjie Ren ,¹ Jianjun He ,¹ and Jianlin Chen¹

¹School of Energy and Power Engineering, Changsha University of Science and Technology, Changsha 410014, China

²Guanxi Key Laboratory of Electrochemical Energy Materials, Guangxi University, Nanning 530004, China

Correspondence should be addressed to Cong Li; liconghntu@csust.edu.cn

Received 4 December 2019; Accepted 10 January 2020; Published 28 January 2020

Guest Editor: Hafiz M. Ali

Copyright © 2020 Jian Chen et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

A novel calculation method of specific surface area of tetrahedral foam metal is established. The expressions of the two basic parameters of the foam metal with respect to porosity and pore size are derived by using the geometrical relationship of this model; consequently, the specific surface area of the metal foam is easily calculated. The theoretical calculation data are compared with the experimental results; it shows that the specific surface area of various porous metals, such as nickel foam and copper foam prepared by electrodeposition and aluminum foam produced by high-pressure infiltration casting, can be well calculated by the formula proposed in this paper. Compared with other similar equations, the calculation results of this method possess lower deviation and greater practicability.

1. Introduction

Facing the double pressure of global environmental pollution and fossil fuel depletion, the development and utilization of renewable clean energy and high-efficient energy storage technology have become the main theme in this century. Lithium ion battery is recognized as an efficient secondary battery. After 30 years of development, lithium ion battery has been widely used in a variety of portable electronic devices. Foam metal is expected to become a potential electrode material for lithium ion batteries due to its excellent properties such as high porosity, high specific surface area, and low bulk density. The excellent performance of porous metals in silencing, separation, filtration, heat exchange, electrochemical processes, and catalytic reaction engineering strongly depends on the structural morphology of surfaces and the specific surface area of porous materials [1–5]. Therefore, the determination of its specific surface area has increasingly attracted the attention of relevant scholars. The specific surface area of a material refers to the surface area per unit volume or unit mass, the former being a volume specific surface area and the latter being a mass specific surface

area. For corrosion performance, it could obtain accurate results by combining the results of surface area and corrosion morphology and can also compare the difference of corrosion behavior between diverse metal foams qualitatively [6]. For fatigue performance, the mechanical properties are directly influenced by two main parameters, including porosity and pore diameter, which determine the surface area of metal foams. Thus, it suggests that there are numerical links between surface area and fatigue performance of porous metal materials [7, 8]. At present, methods for measuring the specific surface area of porous materials include gas adsorption, mercury intrusion, and fluid permeation. Among them, the fluid permeation method is better than the gas adsorption method in terms of the upper and lower limits of measurement and measurement range [9–11]. The mercury intrusion method is a simplified calculation of the specific surface area of the pore body after the pore is assumed to be a uniform cylinder and has a certain error. In reality, the experimental measurement of the specific surface area of materials is often affected by factors such as sample states and equipment conditions, and the theoretical calculations are limited to simple cases where the porosity and pore size

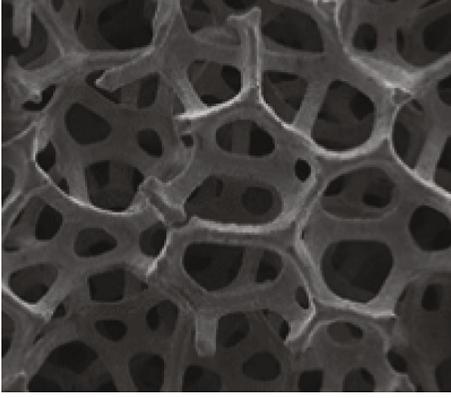


FIGURE 1: Microscopic geometry of foamed copper under electron microscopy.

are known [12]. Therefore, there is an urgent need to develop a specific area measurement or calculation method that is accurate and can be universally applied to practice. Porosity and pore size are basic properties of porous materials and can be determined directly or simply measured [13]. Until now, some researchers have done investigation on the calculation of specific surface area of foam materials, but there are some limitations in practical applications [14, 15]. Liu [16] calculated the specific surface area of the foam metal based on the ideal model of the regular octahedron, but it still needs further improvement in accuracy. Based on the dodecahedron model, Duan et al. [17] provided a method for calculating the specific surface area of foamed metal. However, this method requires measuring the width of the pores first, and the calculation procedure is cumbersome. Based on the above situation, a calculation method which is related to the pore size and porosity for estimating the specific surface area of porous metal based on the tetrakaidecahedron model is proposed.

2. Theoretical Models and Expressions

The high-porosity porous metal can be assumed to be an irregular three-dimensional network structure connected by filamentous metals. The shapes of pores are different, and the struts are interlaced. The directions of the struts in the material are different. However, in an isotropic porous material, the distribution angle of the inner wires is equal. The structural model is simplified to an isotropic high-porosity metal material according to the comprehensive properties of the porous material. An observed microstructure under an electron microscope is shown in Figure 1; it can be seen that the porous material is composed of a large number of small cells; a tetradecahedron structure which is more similar to the actual situation is selected as the basic cell of the metal.

As shown in Figure 2, the surface of the Kelvin tetradecahedron is composed of six regularograms and eight regular hexagons [18], which ensures that the porous material maintains the sameness in the up and down, left and right, and front and back directions. In this paper, the

unit cell structure of the porous material is simplified to a tetradecahedron, and the pore edge is a cylinder. It is assumed that the porosity is θ (%), l is the rib length, r is the radius of the hole, and a is the length of a cube containing the tetradecahedron. The effective specific surface area of the porous metal is the ratio of the surface area sum of tetradecahedral struts to the corresponding porous volume.

Taking Figure 2 as an example, the geometrical method is used to calculate the specific surface area of the unit tetradecahedron. Figure 3 is a projection view of a single cell of a porous material, which is an orthographic projection of a certain angle of the tetradecahedron. The expression of the radius of the tetradecahedron and the radius of the hole can be derived from the geometric relationship shown in the figure.

$$l = \frac{1}{2\sqrt{2}} \cdot a, \quad (1)$$

$$r = \sqrt{\frac{1-\theta}{18\sqrt{2}}} \cdot a. \quad (2)$$

Combine the orthographic projection with the node profile as shown in Figure 4 (the orthographic projection of a node of the unitary tetradecahedron). Using the relevant dimensions to calculate the geometric method, the actual edge length of the porous struts can be expressed as

$$l' \approx l - AB \approx \left(\frac{1}{2\sqrt{2}} - \frac{\sqrt{6}}{9} \sqrt{\frac{1-\theta}{\sqrt{2}\pi}} \right) \cdot a \quad (3)$$

From formulas (2) and (3), the total external surface area of a single tetradecahedron can be calculated as

$$S = \left\{ 6 \left[\frac{\pi(1-\theta)}{\sqrt{2}} \right]^{1/2} - \frac{4\sqrt{6}}{3}(1-\theta) \right\} a^2. \quad (4)$$

Since the inner surface area of the prism is small and the overall influence on the properties related to the porous specific surface area is negligible, in formula (4), the surface area inside the cylindrical rib of a unit cell is ignored. Therefore, the specific surface area of the entire porous structure can be expressed equivalently by the specific surface area of the unit cell tetradecahedron:

$$S_v = \frac{\left\{ 12 \left[(1-\theta)\pi/\sqrt{2} \right]^{1/2} - (8\sqrt{6}/3)(1-\theta) \right\}}{a}. \quad (5)$$

From Figure 5 (forward projection of the tetradecahedron), the projected area of the unit tetradecahedron can be drawn; thus, the equivalent circular aperture can be

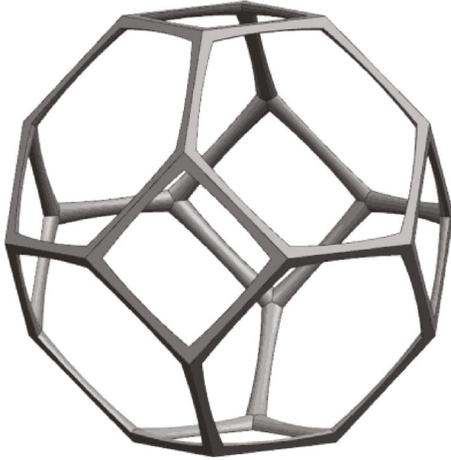


FIGURE 2: Ideal tetrahedral model of foam metal.

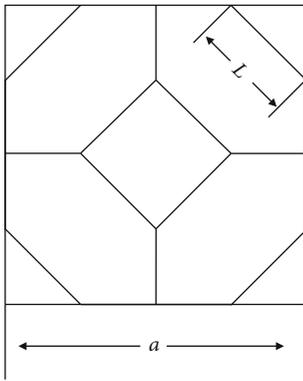


FIGURE 3: Unit cell orthographic projection.

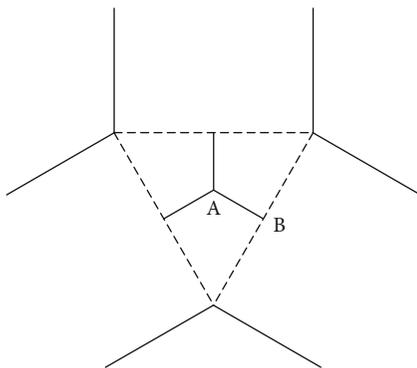


FIGURE 4: Sectional view of the node.

calculated from the projected area, and the relationship between the aperture and the side length a is obtained:

$$S_d = S_o - S_e = \frac{7}{8}a^2 - (2 + 3\sqrt{2}) \cdot r \cdot a - 4r^2. \quad (6)$$

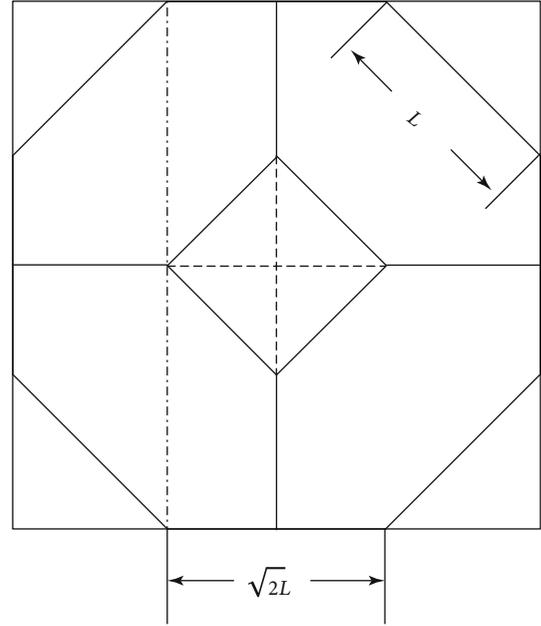


FIGURE 5: Aperture analysis diagram.

Assuming that the projection octahedron equivalent circular aperture is “ d' ,” formula (7) can be obtained:

$$\left(\frac{d'}{2}\right)^2 \pi = S_d. \quad (7)$$

Combined with formula (2), the relationship between d and a can be obtained.

$$d' = \frac{2a}{\pi} \left[\frac{7}{8} - \frac{1 + 2\sqrt{2}}{3\sqrt{\pi}} \cdot (1 - \theta)^{1/2} \right]^{1/2}. \quad (8)$$

Considering that the fluid flows through the inside of the porous body and it is affected by the structure of the porous body, a coefficient “ ε ” is introduced to correct that influence. Normally, the “ ε ” depends on the material and its manufacturing process.

$$d = \varepsilon d'. \quad (9)$$

Through formulas (8) and (9), the relationship between a and d is introduced:

$$a = \frac{d\pi}{2\varepsilon} \left[\frac{7}{8} - \frac{1 + 2\sqrt{2}}{3\sqrt{\pi}} \cdot (1 - \theta)^{1/2} \right]^{1/2}. \quad (10)$$

Combined with formulas (5) and (10), the specific surface area can be simplified and approximated:

$$S_v = \frac{0.596\varepsilon}{d} \left[17.885(1 - \theta)^{1/2} - 6.532(1 - \theta) \right]. \quad (11)$$

TABLE 1: Experimental data and theoretical calculation data of copper foam.

Sample number	1	2	3	4	5	6
Porosity θ (%)	91.5	92.26	92.74	94.57	96.23	96.35
Pore size d (mm)	1.256	1.15	0.755	0.93	0.656	2.385
S_{Ev} (cm ² /cm ³) experimental value	269.07	306.287	456.08	404.43	591.03	165.747
S_{cv} (cm ² /cm ³) calculated value	270.8	301.27	463.9	396.74	598.67	165.55

Since the actual hole edge is not a smooth cylinder, it is an irregular triangular prism type; according to different surface states, a variety of shape changing can be exhibited depending on the material and the preparation process, thereby causing different degrees of surface area increase. Therefore, the above formula should be modified by a coefficient “ δ ” depending on the material and the manufacturing process. If the progress is simplified, then the S_v can be written as follows:

$$S_v = \frac{3.893\epsilon\delta}{d} \left[2.74(1-\theta)^{1/2} - (1-\theta) \right]. \quad (12)$$

For the convenience of calculation, the K is defined as follows:

$$K = 3.893\epsilon\delta. \quad (13)$$

Then, formula (12) can be expressed as

$$S_v = \frac{K}{d} \left[2.74(1-\theta)^{1/2} - (1-\theta) \right]. \quad (14)$$

Among them, “ d (mm)” is the pore size of the porous body, and “ K ” is a constant depending on the material and process of the material. From the experimental perspective, it was proved that the specific surface area increases sharply with the increase of the porosity while the pore diameter of the material does not change much. But formula (14) does not conform to the actual situation. Therefore, a correction factor “ $(1-\theta)^n$ ” is introduced to modify the formula to make it fit for the specific surface area of the actual porous material [13]. Among them, the constant “ n ” is also a material coefficient, which is related to the regularity and geometry of a single unit of porous material, so the formula can be further optimized to

$$S_v = \frac{K}{d} \left[2.74(1-\theta)^{1/2} - (1-\theta) \right] (1-\theta)^n. \quad (15)$$

It is considered that the specific surface area of the porous material is affected by factors such as material, preparation, and geometry. The formula introduces two parameters: “ K ” (material constants related to the material itself and the preparation method) and “ n ” (a constant related to the regularity and geometry of a single unit of porous material). These two material constants are affected by the material preparation process. Theoretically, for the ideal porous materials, the value of “ n ” is zero. It can be deduced from formula (15) that when the porosity of the porous material is kept constant, the

number of unit bodies and the specific surface area decrease as the pore diameter increases. When the pore diameter is kept constant, the number of unit bodies and the specific surface area both increase with the increase of the porosity. However, when the porosity reaches a certain value, the void walls become thinner and thinner until they pass.

This results in a reduction in surface area. Therefore, when the pore diameter is constant, the specific surface area will increase first and then decrease as the pore volume increases.

3. Calculation Results and Analysis

The experimental materials were foamed metal products obtained by electrodeposition and high-pressure percolation casting, respectively. Nickel foam and copper foam with the porosity between 89% and 99% were produced by electrodeposition. Aluminum foam with good connectivity is prepared by high-pressure seepage casting, the porosity is between 73% and 87%, and the pore diameter ranges from 2.68 mm to 2.87 mm.

3.1. Comparison between Experimental Data and Calculated Data. A Micromeritics ASAP 2020 automatic physical and chemical adsorption instrument was used. The instrument can not only measure the single point, multipoint BET specific surface area, Langmuir specific surface area, BJH mesopores, pore distribution, pore size and total pore volume and area, and density function theory (DFT) but also analyze various data such as adsorption heat and average pore size. The working principle of the instrument is the static volumetric method of isothermal physical adsorption. In this experiment, the BET gas adsorption method was used to measure the size parameters of copper foam, including specific surface area and average pore diameter as recorded in Table 1.

Using equation (16), the specific surface area of copper foam can be calculated (take $K = 101.1$, $n = -0.6289$); the result is listed in Table 1.

$$S_v = \frac{101.1}{d} \left[2.74(1-\theta)^{1/2} - (1-\theta) \right] (1-\theta)^{-0.6289}. \quad (16)$$

The comparison between the experimental value and the calculated value is plotted in Figure 6. It can be seen that the calculated results are in line with the experimental data; the deviation is less than 1.2%. The formula presents a high precision.

3.2. Reference Experimental Data and Calculation Results Analysis. The relevant parameters for aluminum foam and nickel foam given in [12, 16] are listed in Tables 2 and 3.

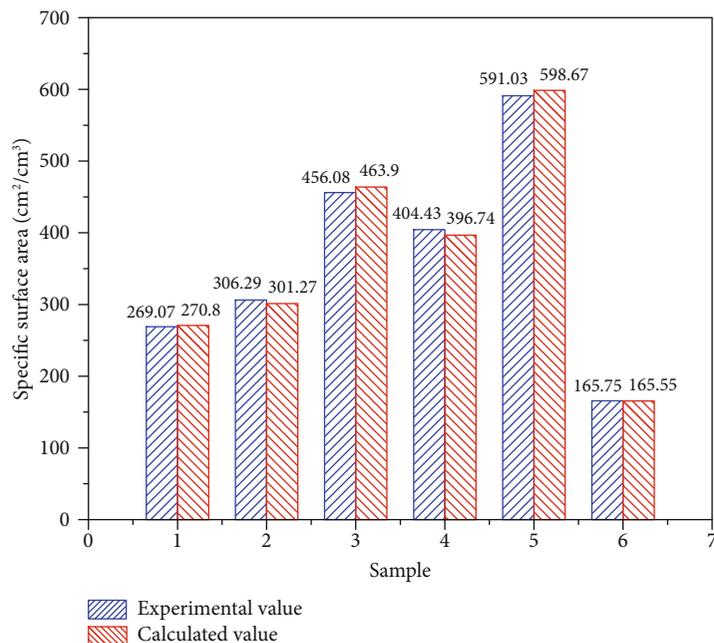


FIGURE 6: Comparison of experimental and calculated values of foamed copper specific surface area.

TABLE 2: Experimental data and theoretical calculation data of aluminum foam.

Sample number	1	2	3	4	5
θ (%)	73.5	76.5	79	82.5	86.5
d (mm)	2.68	2.72	2.75	2.80	2.87
S_{Ev} (cm ² /cm ³) experimental value	15.7	14.7	13.8	12.5	10.7
S_{cv} (cm ² /cm ³) calculated value	16.07	14.91	13.93	12.46	10.6

TABLE 3: Experimental data and theoretical calculation data of foamed nickel.

Sample number	1	2	3	4	5
θ (%)	89.66	92.55	95.79	97.15	98.84
d (mm)	0.5735	0.6008	0.6802	0.7242	0.7378
S_{Ev} (cm ² /cm ³) experimental value	1197.38	1637.48	2649.22	3727.77	9146.05
S_{cv} (cm ² /cm ³) calculated value	1218.898	1646.187	2640.549	3713.126	9150.164

The data are substituted into formula (15) to obtain the corresponding values of n and K , and the calculation result S_{cv} is shown in the last row of the table and compared with the experimental data S_{Ev} . The deviation between the experimental value and the calculated value is plotted in Figure 7.

Using the data given by Reference [16], the specific surface area of porous nickel can be calculated (take $K = 30.03$, $n = -1.4979$).

The result is shown in Table 3. The deviation between the experimental value and the calculated value is plotted in Figure 8.

It can be seen that there is a high consistency between the theoretical results calculated by formula (15) and the actual experimental results. The average deviation of the three sets

of data is 1.2%, and the maximum deviation is less than 1.8%, which proves the accuracy of formula (15).

It can be seen from the comparison of the above data that the formula can be well adapted to the electrodeposition type foam metal and the seepage casting type foam metal, indicating that the formula has good versatility. In the study of this paper, because the metal foam is produced by two different processes, there is a huge difference in its product form. The mesostructure, surface features, nodes, and internal state of the cell body may be quite different, but this formula successfully translates these specific factors which depend on the material type and process conditions into the material constants " δ " and " ε ". So the formula can be applied to different materials with different processes.

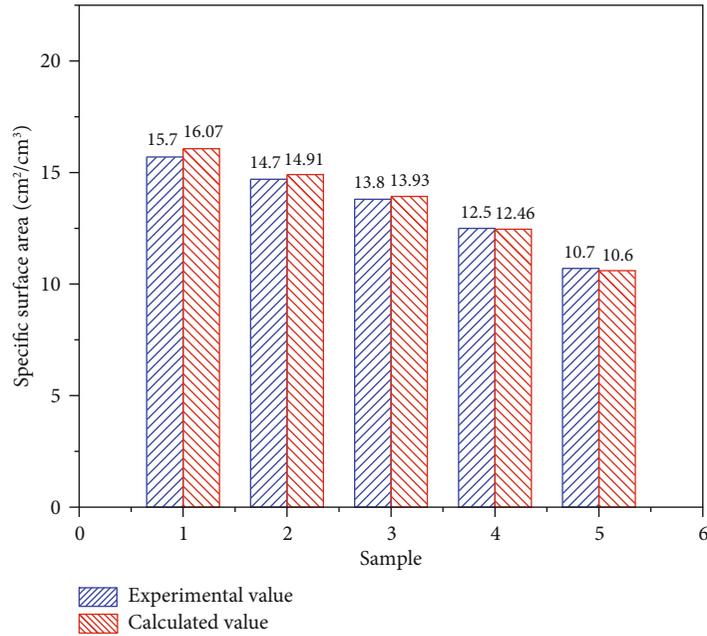


FIGURE 7: Comparison of experimental and calculated values of foamed aluminum specific surface area.

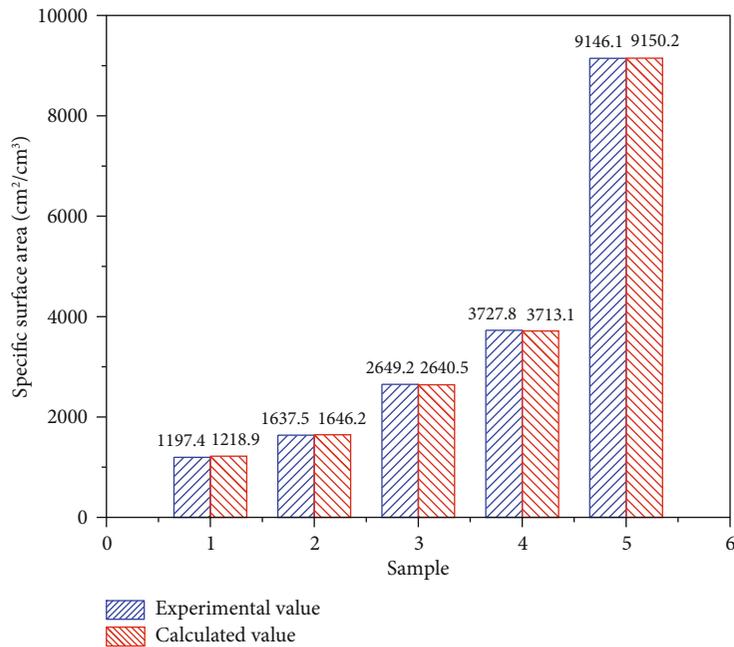


FIGURE 8: Comparison of experimental and calculated values of foamed nickel specific surface area.

The specific values of “*n*” and “*K*” above are obtained by fitting experimental data, the fitting values are used in the formula, and satisfactory results are gained. Both the average deviation and the range of deviation between the calculated and experimental results are very small. Compared with the theoretical octahedral model [16] and the dodecahedron model [17], this model is based on the actual microstructure of foam metal; the calculation results are more accurate.

4. Conclusion

Porosity and pore size are two basic parameters of metal foam. The two parameters of the metal foam are always easy to measure. But sometimes data such as specific surface area is not easy to measure. Using equation (15) herein, the constants *n* and *K* of the material can be obtained easily. Then, a specific equation is established, and the value of the

unmeasured specific surface area of the material can be calculated indirectly from the porosity and the pore diameter.

Considering the factors such as material type and preparation process, the material constant was introduced, and the specific surface area expression of porous metal based on porosity and pore size was established. The specific surface area of the electrodeposited porous metal and the high-pressure percolation cast type porous metal was calculated separately. By comparing with the experimental results, it is found that the theoretical calculation error is small and the applicability of the formula is obviously improved.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare no conflict of interest with respect to this publication.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (Nos. 51471036 and 51675058), Scientific Research Projects of Education Department of Hunan Province (No. 16A002), and Open Foundation of Hunan Provincial Key Laboratory of Energy Efficiency and Clean Utilization (No. 2016NGQ007).

References

- [1] P. S. Liu, T. F. Li, and C. Fu, "Application of porous metal materials," *Journal of Functional Materials*, vol. 32, no. 1, pp. 12–15, 2001.
- [2] J. M. Chen, P. Tan, and J. Y. Wang, "Characterization of specific surface area and pore structure of porous materials by gas adsorption," *Powder Metallurgy Industry*, vol. 21, no. 2, pp. 45–49, 2011.
- [3] C. Li, M. Li, H. Li, J. Chen, and H. Xiao, "Influence of solution treatment on microstructural evolution and mechanical properties of a new titanium alloy," *Kovové materiály- Metallic Materials*, vol. 58, pp. 1–8, 2020.
- [4] C. Li, L. Qin, M. Li, H. Xiao, Q. Wang, and J. Chen, "Influence of deformation strain rate on the mechanical response in a metastable β titanium alloy with various microstructures," *Journal of Alloys and Compounds*, vol. 815, article 152426, 2020.
- [5] C. Li, H. Li, and S. van der Zwaag, "Unravelling the abrasion resistance of two novel meta-stable titanium alloys on the basis of multi-pass-dual-indenter tests," *Wear*, vol. 440–441, article 203094, 2019.
- [6] S. W. Dai, J. Chen, and Y. J. Ren, "Electrochemical corrosion behavior of the copper current collector in the electrolyte of lithium-ion batteries," *International Journal of Electrochemical Science*, vol. 12, pp. 10589–10598, 2017.
- [7] J. Chen, S. Dai, C. Li, W. Li, and Y. Ren, "Effects of pore size on fatigue deformation mechanism of open-cell copper foam at low stress amplitude," *Materials*, vol. 11, no. 9, pp. 1639–1648, 2018.
- [8] J. Chen, X. Li, W. Li et al., "Study on the compression properties and deformation failure mechanism of open-cell copper foam," *Advanced Engineering Materials*, vol. 19, no. 11, pp. 1600861–1600868, 2017.
- [9] P. S. Liu, "Method for determination of specific surface area and pore morphology of porous materials," *Rare Metal Materials and Engineering*, vol. 35, no. S2, pp. 25–29, 2006.
- [10] H. Wang, X. P. Song, and J. J. Liu, "Research progress on specific surface area and pore structure standard materials of porous and highly dispersed materials," *China Powder Science and Technology*, vol. 14, no. 3, pp. 52–55, 2008.
- [11] X. H. Liu, "Experimental study on magnetic properties of porous foam metal and its influence on magnetic field," *Foundry Technology*, vol. 32, no. 6, pp. 815–817, 2011.
- [12] L. Ma and D. He, "Fabrication and pore structure control of new type aluminium foams," *Chinese Journal of Material Research*, vol. 8, no. 1, pp. 11–17, 1994.
- [13] Y. Ding, "Nanoporous metal: a new energy nanomaterial," *Journal of Shandong University (Natural Science)*, vol. 46, no. 10, pp. 121–133, 2011.
- [14] S. J. Zhuang, "A new probe into the calculation method of specific surface area of porous solids," *Chinese Journal of Chromatography*, vol. 4, no. 1, pp. 89–92, 1986.
- [15] Y. Guan, Q. L. Sun, and X. Y. Wu, "Improvement of measurement and calculation methods for specific surface area and pore size distribution," *Acta Chimica Sinica*, vol. 48, no. 5, pp. 424–430, 1990.
- [16] P. S. Liu, "A new method for calculating the specific surface area of porous metal foams," *Philosophical Magazine Letters*, vol. 90, no. 6, pp. 447–453, 2010.
- [17] D. L. Duan, R. L. Zhang, X. J. Ding, and S. Li, "Calculation of specific surface area of foam metals using dodecahedron model," *Materials Science and Technology*, vol. 22, no. 11, pp. 1364–1367, 2006.
- [18] Y. Q. Tu, L. L. Liu, and J. F. Wan, "Improvement of the tetradecahedral model of closed-cell foamed aluminum material," *Chinese Journal of Computational Mechanics*, vol. 27, no. 2, pp. 275–279, 2010.