Simulation study on tribological characteristics of magnetic High-Entropy Alloy FeCoNiCrMn

Kai Ren1,2*, Jianjian Chen3, Hao Wang4 and Zhaoming Huang1

1School of Mechanical Engineering, Wanjiang University of Technology, Maanshan, Anhui, 243031, China
2School of Mechanical and Electronic Engineering, Nanjing Forestry University, Nanjing, Jiangsu, 210037, China
3State Grid Suqian Power Supply Company, State Grid, Suqian, 223899, China
4School of Mechanical Engineering, Southeast University, Nanjing, Jiangsu, 211189 China
*Corresponding author’s e-mail: kairen@njfu.edu.cn

Abstract. To study the tribological characteristics of the high-entropy alloy FeCoNiCrMn under MoS2-oil lubrication conditions in detail, physical testing is combined with finite element method. At room temperature, a ball-on-disk contact pair is selected with reciprocating motion of 5 mm. The single-factor tests are carried out with variables of load (10~50 N) and speed (4.167~20.833 mm/s), and the related wear equation is obtained. Through the static friction contact finite element simulation, the stress and deformation of the friction pair are investigated (the error about 1%), which provides a basis for the partial displacement boundary conditions of the dynamic contact simulation; in the dynamic contact friction simulation, changes in contact pressure and friction stress are analyzed at different loads and velocities. Furthermore, the dynamic friction contact pressure is used to optimize the wear equation and increase the correlation coefficient from 0.89 to 0.96.

1. Introduction
Nowadays, novel materials have attracted lots of attentions [1-5]. High-entropy alloys (HEAs) have become the new generation materials science and engineering due to their potential ideal properties [6, 7]. The large-scale application of HEAs is inseparable from multi-disciplinary and multi-field research, including related tribological exploration. The most reliable data on the tribological behavior of friction pairs can be available through extensive wear tests due to the variety and complexity of tribological phenomena [8-10]. However, when it comes to practical problems involved in uneven load distribution and variable loads (such as the service life of spherical plain bearings with woven linings), experimental exploration is not only expensive, but also unsatisfactory [11].

In the past 30 years, with the rapid development of computer technology and tribology, computational tribology has been a branch of tribology with the strong vitality [12, 13]. To solve the more complex configuration and wear modeling under contact conditions, the finite element method (FEM) is a good choice. The wear simulation includes an iterative process in which the local Archard model is solved by the contact pressure and slip distribution obtained by numerical simulation of discrete time increments [14, 15]. Moreover, the wear value calculated at each increment is used to...
update the worn geometry and the process is repeated until the predefined maximum sliding distance is reached.

According to the existed research, the wear numerical model combined with FEM is mainly based on the Archard equation, but it is found that friction and wear simulations for contacting higher pairs rarely occur. Therefore, this study is carried out with ball-on-disk tests, using the method of combining numerical modeling and FEM, and the tribological behavior of HEA is discussed and analyzed.

In this work, the HEA FeCoNiCrMn is prepared by magnetic levitation melting, and MoS$_2$-oil (containing 1 wt% MoS2) serves as the lubricating medium. Under room temperature conditions, with load (10~50 N) and velocity (4.167~20.833 mm/s) as variables, the wear test is designed in single factor with five levels and conducted. The average friction coefficient and wear volume are taken as the test indicators. The Archard wear equation is established with the measured wear results, and the stress and deformation of the FeCoNiCrMn-GCr15 ball-on-disk pair under static and dynamic contact are analyzed by FEM. In addition, the dynamic average friction contact pressure is used to optimize the FeCoNiCrMn wear model.

2. Materials and methods

2.1. Ball-on-disc wear test

Fig.1 exhibits the wear test is performed on a ball-on-disk instrument (HSR-2M, China). The relative motion mode is reciprocating in 5 mm against the GCr15 ($\phi$5 mm) under MoS$_2$-oil lubrication, which is made up of 500N base oil (NB/SH/T 0914-2015) with MoS$_2$ powder in the mass ratio 1 (MoS$_2$):100 (oil).

Figure 1. The schematic diagram of wear test.

Figure 2. 2D schematic diagram of the friction pair, where green is FeCoNiCrMn matrix; red is the wear area.

| Factor | 1   | 2   | 3   | 4   | 5   |
|--------|-----|-----|-----|-----|-----|
| FN (N) | 10  | 20  | 30  | 40  | 50  |
| Vrel (mm/s) | 4.167 | 8.333 | 12.500 | 16.667 | 20.833 |

The wear test plan is shown in Table 1, where the independent variables are load $F_N$ and velocity $V_{rel}$, and the average friction coefficient $f$ and wear volume $\Delta V$ ($mm^3$) are taken as dependent variables. With the contact metal probe attached to HSR-2M, the two-dimensional contour of the wear scar section is collected. Subsequently, the program gives out the wear volume with the section area and the wear scar length (5 mm) by integration. The sections of each wear scar are measured at three distinguished points, and the final $\Delta V$ is calculated in average to reduce the chance error. The friction coefficient is recorded at sampling frequency of 1 Hz.
2.2. Finite element simulation scheme

$\Delta V$ of FeCoNiCrMn (disk)-GCr15 (ball) working under different $F_N$ and $V_{rel}$ is obtained through the wear test. With data processing and model simplification, the Archard wear model of FeCoNiCrMn at room temperature is built.

However, considering that the contact pressure of the spherical disc pair is difficult to measure directly, the static (Hertz) contact model is employed to associate $F_N$ with the contact pressure $P$. Although the fitting result is acceptable, there is still a certain deviation, because the friction pair is actually subjected to the dynamic frictional contact pressure (different from the static pressure $P$) during the movement process. The more accurate contact pressure can be calculated through the dynamic simulation of frictional contact.

Therefore, the fitting accuracy of the Archard wear equation of FeCoNiCrMn is improved with FEM to replace $P$ with the dynamic contact pressure. In detail, through establishing FeCoNiCrMn–GCr15 contact models under different working conditions, static and dynamic structural simulation research are carried out, and the Archard numerical model of FeCoNiCrMn is optimized.

3. Results and discussions

3.1. Establishment of FeCoNiCrMn-GCr15 wear equation

The exponential Archard equation (1) is used as the wear equation, where $\dot{h}$ is the depth wear rate (mm/s); $A$ is the wear coefficient; $P$ (MPa) is the normal pressure in the contact area; $m$ is the pressure index; $V_{rel}$ is the sliding velocity (mm/s); $n$ is the speed index.

$$\dot{h} = AP^nV_{rel}^m$$  \hspace{1cm} (1)

As shown in Fig 2, the overall shape of FeCoNiCrMn wear scar is approximately drawn by partial spherical surface stretching. Given the large difference in the hardness of the material caused by the contact, the cross section of the wear area is simplified reasonably. The wear motion of the pair is reciprocating linearly in 5 mm, and $\Delta V$ can be calculated from equation (2), where $S$ is the wear cross-sectional area marked in red in Fig 2; $L$ is the length of the wear scar area (5 mm).

$$\Delta V = SL$$  \hspace{1cm} (2)

The geometric relationship between the wear area $S$ and the wear depth $h$ can be described by Equation (3), where $\alpha = \cos^{-1}(1-h/r)$; $r$ is the ball radius 2.5 mm.

$$S = \alpha r^2 - (r-h)\sqrt{2rh-h^2}$$  \hspace{1cm} (3)

When equation (2) is combined with equation (3), equation (4) can be obtained to relate $\Delta V$ to $h$.

$$\Delta V/L = r^2\cos^{-1}(1-h/r) - (r-h)\sqrt{2rh-h^2}$$  \hspace{1cm} (4)

According to equation (4), $\Delta V$ and corresponding $h$ under various conditions are presented in Table 2, where $h$ is the initial value of the iteration taken by the zero function.

| Order | $F_N$(N) | $V_{rel}$(mm/s) | $\Delta V$(10^3mm^3) | $h$(10^3mm) |
|-------|----------|----------------|----------------------|-------------|
| 1     | 10       | 12.500         | 8.130                | 6.676       |
| 2     | 20       | 12.500         | 11.10                | 8.218       |
| 3     | 30       | 12.500         | 22.23                | 13.059      |
| 4     | 40       | 12.500         | 27.33                | 14.988      |
| 5     | 50       | 12.500         | 34.43                | 17.485      |
| 6     | 60       | 4.167          | 12.83                | 9.0513      |
| 7     | 70       | 8.333          | 19.87                | 12.11       |
| 8     | 80       | 12.500         | 22.23                | 13.059      |
| 9     | 90       | 16.667         | 27.30                | 14.977      |
| 10    | 100      | 20.833         | 14.17                | 9.6713      |
Considering that the friction pair is in ball-on-disk contact, the Hertz model is applied to calculate the contact pressure \cite{16}. According to Table 3, the numerical relationship between \( P \) and \( F_N \) can be derived, as shown in equation (5).

\[
P = \frac{1}{\pi} \left[ 6F_N \left( \frac{E_1E_2}{\rho \left( 1 - \mu_1^2 \right) E_2 + \left( 1 - \mu_2^2 \right) E_1} \right) \right]^{\frac{1}{3}} = 438F_N^{\frac{1}{3}}
\]

Table 3. Basic Parameters of Contact Materials

| Name        | FeCoNiCrMn | GCr15 |
|-------------|------------|-------|
| Shape       | Disk Ø30 mm x 3 mm | Sphere Ø5 mm |
| Curvature Radius \( R \) (mm) | \( R_1 (\infty) \) | \( R_2 (2.5) \) |
| Poisson ratio \( \mu \) | \( \mu_1 (0.3) \) | \( \mu_2 (0.3) \) |
| Elasticity modulus \( E \) (MPa) | \( E_1 (6.12 \times 10^4) \) | \( E_2 (2.19 \times 10^5) \) |

Based on equation (5), load conditions are converted to the contact pressure of the FeCoNiCrMn-GCr15 pair in the middle of the contact area, as shown in Table 4. Equation (1) indicates the establishment of the wear model also requires the depth wear rate \( \dot{h} \) (mm/s), which is calculated by equation (6), where \( t \) is the wear time of 15 min.

\[
\dot{h} = \frac{h}{t}
\]

Table 4. GCr15-FeCoNiCrMn Contact Pressure

| \( F_N \) (N) | 10  | 20  | 30  | 40  | 50  |
|----------------|-----|-----|-----|-----|-----|
| \( P \) (MPa) | 949.29 | 1196.03 | 1369.11 | 1506.90 | 1623.26 |

To be specific, the solution optimization algorithm is set to Levenberg-Marquardt; the convergence criterion is 1.00E-10; the maximum number of iterations is 1000; the actual output control number is 20; the mode is standard (LM) with general global optimal (repetition number is 50, control The number of iterations is 30, and the number of iterations for convergence judgment is 20). Ultimately, the Archard wear model of FeCoNiCrMn is built in equation (7).

\[
\dot{h} = AP^nV_x = 5.20 \times 10^{-12} P^{2.08}V_x^{0.13}
\]

For equation (7), it is discovered that the correlation coefficient \( R \) is 0.89, indicating the acceptable fitting effect.

3.2 Static contact analysis of FeCoNiCrMn-GCr15

To facilitate the simulation, the symmetrical simplified processing of the contact pair is performed, as shown in Fig 3. The mesh model mainly consists of hexahedral elements, with a small number of tetrahedral elements contained, and there are 4,348,470 nodes and 1,279,737 elements.
In the Mechanical module of Workbench, contact settings are created automatically. Nevertheless, a few necessary alterations are as follows: the contact type is frictionless; the contact behavior is modified to Asymmetric; the hemisphere is the contact surface, and the disk surface is the target. The bottom surface A of the disk is fixed, the displacement freedom of the B surface of the ball and the C surface of the disk in the X direction are constrained, and the freedom of the D surface of the ball and the E surface of the disk in the Z direction are restricted (Fig 3). Since the model is 1/4 symmetrically simplified, the applied force is 1/4 of $F_N$ along the negative direction of Y (the normal direction of the F surface). Moreover, the loading method is linear within 1 s.

Fig 4 depicts contact pressure distribution diagram. The series of static analysis results show that with the increase of load (2.5~12.5 N), the contact pressure increases from 939.49 MPa to 1632.9 MPa. The high-stress area gradually expands, which appears as the expansion of the red area in the pressure cloud. Thus, it is evident that the previous simplified processing of the model and the division of the grid are reasonable.

3.3 Transient structural analysis of FeCoNiCrMn-GCr15

The tested disk sample is simplified as a 20×10×3 mm cuboid and the ball model is a hemispherical ball (Ø5 mm). The models are divided with adaptive method, and the fine-level correlation center and span angle center are selected. Meanwhile, the contact surface element refinement level is set to 2, with 197,342 nodes and 125,812 elements generated.

The schematic diagram of boundary conditions for the transient structure analysis is displayed in Fig 5, where label A refers to the disk bottom limited in the Y and Z directions; label B represents the side of the disk with the X direction restricted in the displacement of -5 mm; label C is on behalf of the hemisphere plane with the X and Z freedom constrained, and the Y displacement is defined according to different loads (corresponding to the F surface displacement in Table 6).

The contact pair property is frictional, and several specific settings are as follows: (1) The option to automatically update the connection relationship is turned off to avoid overwriting APDL when updating the model during program calculation; (2) The disk surface is selected as the target surface and the ball surface is the contact; (3) The contact behavior is defined as asymmetric contact, Augmented Lagrange algorithm is adopted, and the stiffness is updated in each iteration [17].

With regard to five curves in Fig 6(a), the 0~0.2 s interval corresponds to the slow loading phase, and the pressure curve appears smooth; the 0.2~0.6 s phase is the friction motion phase, and the contact pressure experiences small oscillations. In order to better evaluate the transient contact pressure, the pressure values of all the calculation points in motion phase are extracted, and the average value is taken as the dynamic friction contact pressure.

Fig 6 (b) exhibits that when $F_N$ is 10~50 N, the frictional stress is concentrated at 150~300 MPa. In general, as $F_N$ increases, the contact pressure exerts an upward trend, and the frictional stress increases first (10~40 N) and then slightly decreases (40~50 N).
Table 5 illustrates the key numerical results, where the dynamic friction contact pressure and frictional stress correspond to the average calculated value during the oscillation phase in Fig 6 (a) and (b) respectively. By comparing the static theoretical pressure and the pressure value of 0.2 s in the transient structural analysis, it can be found that the error between the two is about 3%~5%. Therefore, dynamic friction contact pressure and frictional stress obtained from this transient simulation are satisfactory. Besides, as the load increases, the dynamic friction contact pressure rises steadily, but the growth rate slows down; the frictional stress puts up a phased rise mainly divided into three sections (10 N, 20~30 N and 40~50 N).

### Table 5. Contact Pressure (Theoretical and Simulated) And Frictional Stress Under Different Loads

| $F_N$ (N) | Theoretical pressure (MPa) | Simulated pressure _0.2 s (MPa) | Dynamic friction contact pressure (MPa) | Frictional stress (MPa) |
|-----------|-----------------------------|----------------------------------|----------------------------------------|------------------------|
| 10        | 943.410                     | 967.80                           | 1015.138                               | 169.030                |
| 20        | 1188.622                    | 1228.0                           | 1285.862                               | 214.477                |
| 30        | 1360.632                    | 1389.3                           | 1436.804                               | 219.554                |
| 40        | 1497.569                    | 1584.5                           | 1637.774                               | 259.724                |
| 50        | 1613.208                    | 1683.8                           | 1732.139                               | 246.129                |

Similarly, the contact pressure for transient structural simulation at various velocities (4.167~20.833 mm/s) are seen in Fig 7 (a), suggesting that as $V_{rel}$ increases, the contact pressures hardly distinguish each other, basically maintained around 1445 MPa. Note that the contact pressure at 0.2 s in Fig 7 (a) is 1388 MPa, and the theoretical pressure at 30 N is 1360 MPa, demonstrating that the dynamic friction contact simulation under diversified velocities is more accurate relatively. Table 9 mentions that the dynamic friction contact pressure rises from 1436.804 MPa to 1450.500 MPa with $V_{rel}$ increased, but the change is not obvious.

### Figure 7. Time history of transient contact pressure and frictional stress under different velocities with the load of 30 N.

Fig 7 (b) introduces that the frictional stress experienced by the contact pair declines with $V_{rel}$ increased, ranging from 150 MPa to 350 MPa. Further, for the 4.167~12.500 mm/s stage, the velocity increase significantly impacts on reducing the frictional stress; when the interval of 12.500~20.833 mm/s is reached, the phenomenon that the frictional stress decreases as the velocity increases weakens. In accordance with Table 6, the frictional stress is the maximum value of 323.382 MPa when the velocity is 4.167 mm/s; the frictional stress is minimized (171.035 MPa) at 20.833 mm/s.

### Table 6. Contact Pressure Simulated and Frictional Stress Under Different Velocities

| $V_{rel}$ (mm/s) | Simulated pressure _0.2 s (MPa) | Dynamic friction contact pressure (MPa) | Frictional stress (MPa) |
|------------------|----------------------------------|----------------------------------------|------------------------|
| 4.167            | 1389.3                           | 1436.804                               | 323.382                |
| 8.333            | 1389.0                           | 1445.545                               | 276.269                |
| 12.500           | 1388.6                           | 1446.555                               | 219.554                |
| 16.667           | 1388.5                           | 1447.819                               | 203.470                |
| 20.833           | 1388.3                           | 1450.500                               | 171.035                |
4. Conclusion
Static contact analysis confirms that a mesh model consisting of 4,348,470 nodes and 1,279,737 elements has been utilized to extract contact pressure simulation results with an error of about 1%. Further, reliable data support is provided for the conversion of boundary conditions (force to displacement) in the transient structural analysis.

Under specifically different loads or velocities, the contact pressure in the dynamic friction phase is slightly greater than that at the moment of the static loading completed; as the load increases (with the velocity 12.500 mm/s), both dynamic friction contact pressure and frictional stress rise. For the working condition where the load is 30 N and the velocity is increasing, the dynamic friction contact pressure fluctuates mildly, and the frictional stress drops accordingly.

Through data analysis and reorganization of dynamic friction contact pressure and other essential parameters, the modified wear model is constructed, improving the correlation coefficient R from 0.89 to 0.96.

Conflicts of interest
There are no conflicts to declare.

Acknowledgment
This work was supported by the Open Fund Project of Maanshan Engineering Technology Research Center of Advanced Design for Automotive Stamping Dies (Grant number: QMSG202105).

References
[1] K. Ren, X. Liu, S. Chen, Y. Cheng, W. Tang, G. Zhang, Adv. Funct. Mater., (2020) 2004003.
[2] M. Sun, U. Schwingenschlögl, Chem. Mater., 32 (2020) 4795-4800.
[3] J. Li, Z. Huang, W. Ke, J. Yu, K. Ren, Z. Dong, Journal of Alloys and Compounds, 866 (2021).
[4] M. Sun, U. Schwingenschlögl, Advanced Energy Materials, (2021).
[5] Z. Zheng, K. Ren, Z. Huang, Z. Zhu, K. Wang, Z. Shen, J. Yu, Semiconductor Science Technology, (2021) 075015.
[6] Y. Ye, Q. Wang, J. Lu, C. Liu, Y. Yang, Materials Today, 19 (2016) 349-362.
[7] H. Wang, K. Ren, J. Xie, C. Zhang, W. Tang, Industrial Lubrication and Tribology, 72 (2019) 665-672.
[8] Y. Ye, C. Liu, H. Wang, T. Nieh, Acta Materialia, 147 (2018) 78-89.
[9] Y. Yu, J. Wang, J. Li, J. Yang, H. Kou, W. Liu, Journal of Materials Science & Technology, 32 (2016) 470-476.
[10] S. Kumar, A. Patnaik, A.K. Pradhan, V. Kumar, Journal of Materials Research, 34 (2019) 841-853.
[11] X. Shen, Y. Liu, L. Cao, X. Chen, Journal of materials research and technology, 1 (2012) 8-12.
[12] J. Archard, in, New York, NY, 1980.
[13] R.D. Cook, Concepts and applications of finite element analysis, John Wiley & Sons, 2007.
[14] V. Hegadekatte, N. Huber, O. Kraft, Modelling and Simulation in Materials Science and Engineering, 13 (2004) 57.
[15] V. Hegadekatte, S. Kurzenhäuser, N. Huber, O. Kraft, Tribology international, 41 (2008) 1020-1031.
[16] K.L. Johnson, K.L. Johnson, Contact mechanics, Cambridge university press, 1987.
[17] G.R. Bhashyam, Ansys, Inc, 1 (2002) 39.