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Calculated electromigration wind force in molybdenum disilicide

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Kurzfassung

Mit Hilfe von Machine Learning (random forest) konnte die Größe der Windkraft-Komponente der effektiven Ionenladung der Elektromigration in Molybdändisilizid für verschiedene Atomsorten bestimmt werden.
Es ist zu erkennen, dass alle Atomsorten einen vergleichsweise kleinen Wert von Z^*_{wind} ≈-1 für diese Komponente aufweisen. Da in der Regel die direkte Komponente einen wesentlich kleineren Beitrag zur effektiven Ionenladung ergibt als die Windkraft-Komponente, kann die hier bestimmte Windkraft-Komponente als Näherung der effektiven Ionenladung.

Abstract

Using a machine learning approach with a random forest model the value of the wind force component of the effective ion charge of electromigrating ions in molybdenum disilicide was estimated for several ion species. The value of Z^*_{wind} ≈-1 is small compared to effective ion charges in other host materials. Because of the direct component having a small contribution to the effective ion charge compared to the wind force, the wind force component of the effective ion charge can be used as approximation for the effective ion charge itself.

1 Introduction

Because of chip sizes decreasing and current densities increasing electromigration becomes more important.
Electromigration is the movement of atoms in an electrically conductive material caused by current through the material.
Molybdenum disilicide ($MoSi_2$) and electromigration therein are of great importance because of the widespread use of the material in macroscopic and microscopic heating devices.
$MoSi_2$ is often used in microheaters because of its high melting point and its CMOS compatibility. The high melting point of $MoSi_2$ is the reason it has been considered to be immune to electromigration for a long time. This is the reason electromigration in the material has not been investigated thoroughly, despite several researchers proving the existence of electromigration phenomena in $MoSi_2$ [1].

1.1 Electromigration

The electromigration force $\vec{F}$ on an ion caused by the electric field $\vec{E}$ can be described as
$\vec{F} = Z^* e\vec{E} = (Z^*_{dir} + Z^*_{wind})e\vec{E}$.
With Z^* being the effective ion charge and e being the elemental charge.
$Z^* = Z^*_{dir} + Z^*_{wind} = Z^*_{dir} + K/\rho$,
with K depending on the material but being independent of the temperature [2].
For most materials Z^*_{dir} is small compared to Z^*_{wind} [2]. This allows the use of Z^*_{wind} as an approximation for Z^*in these materials
$Z^* \approx Z^*_{wind} = K/\rho$.
Because of the experimental challenges of the determination of Z^* simulations using density functional theory or machine learning might give adequate results much faster.

2 Method

In this work a machine learning approach was performed using the Materials Simulation Toolkit for Machine Learning (MAST-ML) [3] to determine K for a plethora of atoms in $MoSi_2$. The path averaged K values of [2] have been used as dataset because of K being available for a multitude of atom combinations.
Care was taken not to have multiples of a data point and to exclude data points in which the crystal structure mentioned in [2] would not have matched the crystal structure of the feature generation of the elemental feature generator. This resulted in 139 data points being used. The elemental properties were constructed using the Materials Agnostic Platform for Informatics and Exploration (MAGPIE) approach.
The elemental feature generator has been used to generate features of the combination of impurity and host material to give composition averages, arithmetic averages, the minimum, the maximum, and the differences between the two of them.
In the first runs of the machine learning algorithm the selection of the input parameters of the sequential forward selection algorithm (SFS) showed the melting temperature being an important parameter. The elemental feature generator cannot give an adequate melting temperature of $MoSi_2$, therefore the melting temperature of the host material, the electromigrating ion and the arithmetic average thereof were added as features.
The data was cleaned using imputation of the median for missing values.
Normalization was done to standardize the data prior to fitting. After normalization the mean of each feature is 0 and the standard deviation of the feature is 1.

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A random forest regressor was chosen using 125 estimators employing an ensemble model feature selector including SFS.
The feature learning curve (Figure 1) showes a decrease of the mean absolute error until the number of 7 features is met.

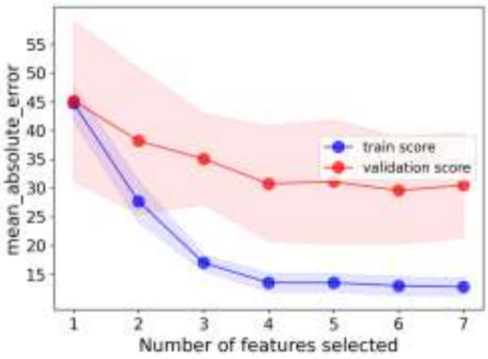

Figure 1 Feature learning curve.

Therefore, the number of 7 features was selected in the ensemble model feature selector. The features used are ranked according to their importance in Table 1.

Feature	Importance
IsMetalloid_difference	0.12795
Host-Melting-Temperature	0.09682
HeatFusion_max_value	0.05481
CovalentRadius_min_value	0.04667
ThermalConductivity_max_value	0.02988
NUnfilled_min_value	0.02681
Polarizability_min_value	0.02373

Table 1 Selected features and their importance.

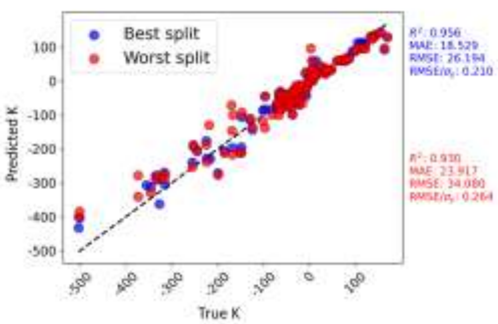

Figure 2 5-fold CV test.

The ρ values used in [2] to calculate Z^*_{wind} are the specific resistivities of polycrystalline materials at the temperature of 473 K.
For $MoSi_2$ a value of ρ=154.13 µΩ cm has been determined due to measurements of the resistance at 473 K and was used in the calculation of Z^*_{wind}.

Electromigrating material	Z^*_{wind}
Sc, Ti, V, Cr, Mn, Fe, Ga, Ge, Sr, Y, Zr, Nb, Mo, Tc, Ru, Cd, In, Sn, Ba, Hf, Ta, Re, Os, Hg, Tl, Pb, Ra, Rf, Db, Sg, Bh, Hs, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Yb, Lu, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, No, Lr	-1.0029
Li, Na, K, Rb, Cs, At, Fr, Tm, Md	-1.0141
He, B, Ne, Ar, Zn, Kr, Pd, Xe, Rn	-0.9885
Ni, Te, Pt, Po, Ds, Er, Fm	-0.9630
Co, Sb, Ir, Mt, Ho, Es	-1.0265
H, F, Cl, Br, I	-0.9985
P, As, Rh, Bi	-1.018
O, S, Se	-0.9553
Be, Ca	-1.0234
Ag	-1.1594
Au	-1.1398
Cu	-1.1338
Al	-1.066
Si	-1.0368
W	-1.0009
Mg	-0.9866

Table 2 Z^*_{wind} determined by machine learning of K.

3 Conclusion

The host melting temperature being one of the most important features influencing the effective ion charge is well known. The electrical conductivity is known to influence the effective ion charge. Instead of the electrical conductivity the SFS identified the thermal conductivity to be of importance. This is because of the strong correlation between the two of them.
The values of Z^*_{wind} being close to -1 is plausible.
Typical values of Z^* are either in the same range or one or two magnitudes larger.
The value of Z^*_{wind} being comparatively small in $MoSi_2$ might explain $MoSi_2$ to have been considered immune to electromigration.

4 Literature

[1] Zehe, A.; Ramirez, A.: Electromigration of aluminium through quasi bamboo-like grain blocked silicide interconnects, Crystal research and technology 35, 5 (2000), S. 557-562

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[3] Jacobs, R., Mayeshiba, T., Afflerbach, B., Miles, L., Williams, M., Turner, M., Finkel, R., Morgan, D.: The Materials Simulation Toolkit for Machine Learning (MAST-ML): An automated open source toolkit to accelerate data- driven materials research, Comp. Mat. Sci. 175 (2020), 109544