Supplementary Information

Assessment of the interatomic potentials of beryllium for mechanical properties

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Supplementary Tables

Table S1. The parameters of MEAM type potential developed for beryllium.

r_{cut}	α	$\beta^{(0)}$	$\beta^{(1)}$	$\beta^{(2)}$	$\beta^{(3)}$
3.5	3.8501	0.24826	0.004161	0.33524	3.8426×10^{-7}
r_e	E_c	A	$t^{(0)}$	$t^{(1)}$	$t^{(2)}$
2.2433361	3.42	1.1801	1.0	4.5561	21.956
$t^{(3)}$	δ	C_{min}	C_{max}		
-10.234	0.01	1.1	1.5		

Table S2. The parameters of Tersoff type potential developed for beryllium.

R (Å)	D (Å)	A	B	λ_1	λ_2	n
2.685	0.223	367.830	13.915	3.193	1.026	1.0
β (Å^{-1})	m	λ_3	c	d	γ	$\cos\theta_0$
1.0	1.0	1.7	32.328	0.053	4.787×10^{-7}	-0.827

Table S3. The parameters of the Finnis-Sinclair type potential developed for beryllium.

r_{a1}	r_{a2}	r_{a3}	r_{a4}	r_{a5}	r_{a6}	r_{a7}
2.0400000	1.7407111	1.3816634	1.2278749	1.0400000	0.97352665	0.96379139
A_1	A_2	A_3	A_4	A_5	A_6	A_7
0.8975540	-2.0922508	-6.9015384	18.6591697	55.5572581	50.0000000	100.0000000
r_{b1}	r_{b2}	r_{b3}	r_{b4}	r_{b5}	m	n
2.0400000	1.7233905	1.4095758	1.2242095	1.0408000	5	7
B_1	B_2	B_3	B_4	B_5	A	
2.7114616	-5.9662845	-19.6955993	57.1589316	188.8640451	0.00638918	

Table S4. Effect of void size of spherical void on the mechanical performance of beryllium subject to uniaxial tension. The interatomic potential used is the MEAM potential.

Void-embedded	**0**	**12**	**56**	**159**	**407**
Tensile toughness(J/m^3)	1.559	1.455	1.279	0.995	0.942
Young's modules(GPa)	294.8	294.6	294.0	293.6	289.2
Fracture stress(GPa)	25.12	24.53	23.38	20.68	19.806
Fracture strain	0.109	0.105	0.098	0.086	0.084
Void-embedded	**775**	**1339**	**2114**	**3148**	**4505**
Tensile toughness(J/m^3)	0.959	0.869	0.819	0.743	0.666
Young's modules(GPa)	281.9	272.9	264.3	250.7	236.6
Fracture stress(GPa)	19.77	18.27	17.61	16.31	14.75
Fracture strain	0.086	0.083	0.082	0.08	0.078

Table S5. Effect of temperature on the mechanical performance of beryllium subject to uniaxial tension. The interatomic potential used is the MEAM potential.

Temperature(K)	**150**	**300**	**450**	**600**
Tensile toughness(J/m^3)	1.361	0.959	0.622	0.360
Young's modules(GPa)	285.4	281.9	281.0	274.6
Fracture stress(GPa)	23.86	19.77	17.50	11.62
Fracture strain	0.103	0.086	0.069	0.052

Table S6. Effect of void size of spherical void on the mechanical performance of beryllium subject to uniaxial tension. The interatomic potential used is the Tersoff potential.

Void-embedded	**0**	**12**	**56**	**159**	**407**
Tensile toughness(J/m³)	1.986	1.510	1.336	1.199	1.091
Young's modules(GPa)	192.1	191.7	189.2	190.6	186.7
Fracture stress(GPa)	37.77	33.95	31.87	29.42	27.29
Fracture strain	0.121	0.108	0.103	0.099	0.096
Void-embedded	**775**	**1339**	**2114**	**3148**	**4505**
Tensile toughness(J/m³)	1.038	1.008	0.995	0.871	0.870
Young's modules(GPa)	188.3	176.5	172.7	164.5	155.9
Fracture stress(GPa)	25.92	25.27	24.51	22.26	21.75
Fracture strain	0.095	0.095	0.096	0.093	0.095

Table S7. Effect of temperature on the mechanical performance of beryllium subject to uniaxial tension. The interatomic potential used is the Tersoff potential.

Temperature(K)	**150**	**300**	**450**	**600**
Tensile toughness(J/m³)	1.157	1.038	0.948	0.853
Young's modules(GPa)	185.0	188.3	193.1	202.6
Fracture stress(GPa)	29.78	25.92	23.61	21.21
Fracture strain	0.102	0.095	0.089	0.083

Table S8. Effect of void size of spherical void on the mechanical performance of beryllium subject to uniaxial tension. The interatomic potential used is the Finnis-Sinclair potential.

Void-embedded	**0**	**12**	**56**	**159**	**407**
Tensile toughness(J/m^3)	1.035	1.071	0.993	0.907	0.844
Young's modules(GPa)	306.2	310.7	298.1	300.1	299.8
Fracture stress(GPa)	19.40	19.41	19.31	18.78	18.19
Fracture strain	0.089	0.091	0.087	0.083	0.08
Void-embedded	**775**	**1339**	**2114**	**3148**	**4505**
Tensile toughness (J/m^3)	0.790	0.733	0.709	0.695	0.689
Young's modules (GPa)	296.5	284.2	275.0	261.2	252.0
Fracture stress (GPa)	17.59	16.94	16.39	15.63	14.95
Fracture strain	0.078	0.076	0.076	0.077	0.079

Table S9. Effect of temperature on the mechanical performance of beryllium subject to uniaxial tension. The interatomic potential used is the Finnis-Sinclair potential.

Temperature (K)	**150**	**300**	**450**	**600**
Tensile toughness (J/m^3)	0.796	0.790	0.757	0.687
Young's modules (GPa)	280.3	296.5	299.1	296.0
Fracture stress (GPa)	18.31	17.59	16.74	15.91
Fracture strain	0.074	0.078	0.076	0.072