

Supplementary Materials: The following are available online at <http://www.mdpi.com/2075-4701/10/7/863/s1>,. Thermodynamic calculation process of desulphurization are as follow. Table S-1 S-2 and S-3 are the composition of tested steels, interaction coefficients and chemical equations of reaction used for the calculation.

Table S1. Chemical composition of tested steels for calculation/%.

	C	Si	Mn	P	S	Al	T.O	N	Ti	Fe
Base metal	0.06	0.24	1.44	0.01	0.008	0.005	0.008	0.004	0.014	Bal.

Table S2. First order interaction coefficients of elements in 1873 K.

	C	Si	Mn	P	S	Al	O	N	Ti
Mg	0.15	0.09	0	0	-1.38	-0.12	-430	0	0
Ce	-0.077	0	0.13	1.746	-39.8	-2.25	-5.03	-6.612	0
S	0.11	0.063	-0.026	0.029	-0.028	0.035	-0.27	0.01	-0.072
O	-0.45	-0.131	-0.021	0.07	-0.133	-3.9	-0.20	0.057	-0.6

Table S3. Chemical equation of reaction ($\Delta G^\theta = A + BT$) [16,19].

	A	B	lgK ^θ
Ce2O2S(s)=2[Ce]+2[O]+[S]	1351400	-331	-20.396
CeS(s)=[Ce]+[S]	422100	-120.38	-5.4828
Ce2S3(s)=2[Ce]+3[S]	1072840	-327.72	-12.799
Ce3S4(s)=3[Ce]+4[S]	1493010	-438.9	-18.709
MgS(s)=[Mg]+[S]	537258.5	-205.77	-4.2343

According to Wagner model:

$$\lg f_i = \sum_1^n e_i^j [\%j] \quad (S-1)$$

Table 4. Activity coefficients of elements in 1873 K.

i	Mg	Ce	S	O
lgfi	-3.42104	-0.1963	-0.0186	-0.1183

For Ce₂O₂S,

$$\lg K^\theta = \lg \frac{a_{Ce}^2 \cdot a_O^2 \cdot a_S}{a_{Ce_2O_2S}} \quad (S-2)$$

$$a_i = f_i \cdot [\%i] \quad (S-3)$$

$$a_{Ce_2O_2S} = 1 \quad (S-4)$$

Bring (S-3), (S-4) into (S-2),

$$2 \times \lg[\%Ce] + \lg[\%S] + 14.95 = 0 \quad (S-5)$$

Similarly,

For CeS,

$$\lg[\%Ce] + \lg[\%S] + 5.268 = 0 \quad (\text{S-6})$$

For Ce₂S₃,

$$2 \times \lg[\%Ce] + 3 \times \lg[\%S] + 12.35 = 0 \quad (\text{S-7})$$

For Ce₃S₄,

$$3 \times \lg[\%Ce] + 4 \times \lg[\%S] + 18.05 = 0 \quad (\text{S-8})$$

For MgS,

$$\lg[\%Mg] + \lg[\%S] + 0.795 = 0 \quad (\text{S-9})$$

Desulphurization curves of Ce and Mg were drawn based on equation (S-5) to (S-9) and shown in Figure 2(b).