

Table 2. Structure refinements of ilmenite-hematite samples as a function of temperature and composition

ilm80

20	5.07860(4)	13.9850(2)	0.009(1)	0.978(3)	0.35500(4)	0.15285(44)	0.3160(1)	0.0188(1)	0.2462(0)	0.0062(1)	0.0067(1)	2.60
200	5.09297(4)	14.0123(2)	0.007(1)	0.982(3)	0.35543(5)	0.15460(48)	0.3163(1)	0.0189(1)	0.2461(0)	0.0097(2)	0.0103(2)	2.42
400	5.10303(4)	14.0381(2)	0.004(1)	0.990(3)	0.35585(5)	0.15365(50)	0.3162(1)	0.0189(1)	0.2461(0)	0.0119(2)	0.0127(2)	2.41
500	5.10853(5)	14.0513(2)	0.012(1)	0.970(3)	0.35612(5)	0.15411(58)	0.3162(2)	0.0183(1)	0.2462(0)	0.0128(2)	0.0142(2)	2.30
600	5.11414(5)	14.0618(3)	0.018(1)	0.955(3)	0.35632(5)	0.15582(70)	0.3162(2)	0.0180(2)	0.2461(1)	0.0140(2)	0.0157(2)	2.32
700	5.12089(5)	14.0738(3)	0.025(1)	0.937(3)	0.35656(6)	0.15756(88)	0.3163(2)	0.0179(2)	0.2462(1)	0.0155(3)	0.0170(2)	2.38
800	5.12782(5)	14.0881(3)	0.035(1)	0.912(3)	0.35690(7)	0.15973(127)	0.3163(2)	0.0177(2)	0.2464(1)	0.0175(3)	0.0188(3)	2.44
900	5.13517(5)	14.1015(3)	0.051(2)	0.873(5)	0.35722(7)	0.16987(288)	0.3160(2)	0.0172(2)	0.2466(1)	0.0206(4)	0.0212(4)	2.44
1000	5.14371(6)	14.1160(3)	0.097(2)	0.757(5)	0.35718(11)	0.12743(177)	0.3153(2)	0.0173(3)	0.2471(1)	0.0225(4)	0.0230(4)	2.51
1100	5.15034(7)	14.1150(4)	0.172(2)	0.570(5)	0.35755(20)	0.13843(101)	0.3140(3)	0.0153(4)	0.2476(1)	0.0255(5)	0.0240(5)	2.52
1150	5.15471(8)	14.1101(4)	0.293(4)	0.267(10)	0.35856(58)	0.14159(110)	0.3126(4)	0.0121(6)	0.2489(3)	0.0275(6)	0.0239(5)	2.55
1175	5.15674(8)	14.1119(4)	0.40	0.0	0.35866(9)	0.14134(9)	0.3062(2)	0.0	0.25	0.0312(7)	0.0282(6)	2.43
1200	5.15864(8)	14.1154(4)	0.40	0.0	0.35865(10)	0.14135(10)	0.3063(2)	0.0	0.25	0.0328(7)	0.0296(6)	2.46
1225	5.16056(8)	14.1197(4)	0.40	0.0	0.35881(9)	0.14119(9)	0.3067(2)	0.0	0.25	0.0338(7)	0.0306(6)	2.33
1250	5.16252(8)	14.1238(4)	0.40	0.0	0.35903(10)	0.14097(10)	0.3066(2)	0.0	0.25	0.0343(8)	0.0307(6)	2.44
1275	5.16455(8)	14.1290(4)	0.40	0.0	0.35903(9)	0.14097(9)	0.3067(2)	0.0	0.25	0.0341(7)	0.0306(6)	2.26
1300	5.16651(8)	14.1343(4)	0.40	0.0	0.35916(10)	0.14084(10)	0.3065(2)	0.0	0.25	0.0360(8)	0.0319(7)	2.28

Table 2

1325	5.16878(9)	14.1419(5)	0.40	0.0	0.35921(10)	0.14079(10)	0.3063(2)	0.0	0.25	0.0362(9)	0.0322(7)	2.42
1200	5.15887(9)	14.1177(5)	0.40	0.0	0.35893(10)	0.14107(10)	0.3051(2)	0.0	0.25	0.0325(8)	0.0288(7)	2.57
1000	5.14063(6)	14.1109(3)	0.088(2)	0.779(5)	0.35755(10)	0.11879(191)	0.3156(2)	0.0175(3)	0.2469(1)	0.0226(4)	0.0233(4)	2.54
800	5.12668(5)	14.0881(3)	0.025(1)	0.937(3)	0.35706(7)	0.15668(103)	0.3161(2)	0.0183(2)	0.2464(1)	0.0182(3)	0.0196(3)	2.52
600	5.11479(5)	14.0610(3)	0.008(1)	0.979(3)	0.35651(6)	0.15451(63)	0.3164(2)	0.0191(2)	0.2462(1)	0.0155(3)	0.0170(2)	2.58

ilm90

20	5.08280(4)	14.0330(2)	0.008(1)	0.982(2)	0.35534(4)	0.1474(2)	0.3170(1)	0.0217(1)	0.24571(4)	0.0072(1)	0.0090(2)	2.84
200	5.09600(5)	14.0605(2)	0.007(1)	0.984(2)	0.35586(5)	0.1482(2)	0.3173(2)	0.0220(1)	0.24575(4)	0.0112(2)	0.0129(2)	2.85
400	5.10589(5)	14.0872(2)	0.004(1)	0.991(2)	0.35623(5)	0.1481(2)	0.3177(2)	0.0222(1)	0.24564(5)	0.0137(2)	0.0151(2)	2.67
500	5.11108(5)	14.1009(3)	0.007(1)	0.984(2)	0.35641(5)	0.1483(2)	0.3178(2)	0.0222(1)	0.24573(5)	0.0142(2)	0.0162(2)	2.66
600	5.11647(5)	14.1142(3)	0.007(1)	0.984(2)	0.35661(5)	0.1485(2)	0.3180(2)	0.0222(2)	0.24573(5)	0.0156(2)	0.0174(2)	2.58
700	5.12214(5)	14.1257(3)	0.013(1)	0.971(2)	0.35678(6)	0.1487(2)	0.3181(2)	0.0221(2)	0.24572(5)	0.0171(3)	0.0187(3)	2.58
800	5.12822(5)	14.1385(3)	0.019(1)	0.958(2)	0.35708(6)	0.1490(3)	0.3187(2)	0.0220(2)	0.24580(6)	0.0184(3)	0.0202(3)	2.60
900	5.13439(6)	14.1543(3)	0.027(2)	0.940(4)	0.35729(7)	0.1489(3)	0.3183(2)	0.0219(2)	0.24598(7)	0.0210(4)	0.0227(3)	2.66
1000	5.14110(6)	14.1682(3)	0.039(2)	0.913(4)	0.35755(9)	0.1496(4)	0.3179(3)	0.0221(2)	0.24622(8)	0.0257(5)	0.0267(5)	2.82
1100	5.14838(7)	14.1799(4)	0.059(2)	0.869(4)	0.35789(11)	0.1502(6)	0.3176(3)	0.0219(3)	0.24646(10)	0.0299(7)	0.0301(6)	2.87
1150	5.15269(8)	14.1826(4)	0.076(2)	0.831(4)	0.35815(13)	0.1498(8)	0.3176(3)	0.0215(3)	0.24672(12)	0.0324(9)	0.0321(8)	2.86
1200	5.15717(8)	14.1827(5)	0.103(2)	0.771(4)	0.35826(14)	0.1525(13)	0.3171(3)	0.0207(3)	0.24701(13)	0.0333(4)	0.0319(4)	2.79
1225	5.15937(8)	14.1813(5)	0.121(2)	0.731(4)	0.35851(14)	0.1579(18)	0.3164(3)	0.0196(3)	0.24726(14)	0.0362(9)	0.0334(9)	2.68
1250	5.16177(9)	14.1776(5)	0.144(3)	0.680(7)	0.35887(14)	0.1726(34)	0.3161(4)	0.0188(4)	0.24719(15)	0.0379(9)	0.0341(9)	2.63
1275	5.16476(8)	14.1728(4)	0.208(3)	0.538(7)	0.35902(23)	0.1296(24)	0.3153(3)	0.0169(4)	0.24735(16)	0.0406(5)	0.0365(3)	2.36
1300	5.16818(9)	14.1649(5)	0.305(4)	0.322(9)	0.35929(53)	0.1372(15)	0.3130(4)	0.0136(6)	0.24793(25)	0.0460(6)	0.0391(4)	2.42
1325	5.17053(10)	14.1645(5)	0.45	0.0	0.36014(14)	0.1399(1)	0.3055(2)	0.0	0.25	0.0496(7)	0.0412(4)	2.43
1350	5.17169(16)	14.1695(8)	0.45	0.0	0.35950(22)	0.1405(2)	0.3034(3)	0.0	0.25	0.0364(10)	0.0257(7)	2.70
1200	5.15389(10)	14.1756(6)	0.093(3)	0.793(7)	0.35814(16)	0.1528(13)	0.3165(4)	0.0218(4)	0.24707(14)	0.0289(5)	0.0264(4)	3.19
1000	5.13707(7)	14.1591(4)	0.030(2)	0.933(4)	0.35760(9)	0.1489(4)	0.3183(3)	0.0229(2)	0.24609(9)	0.0270(6)	0.0274(5)	3.00
800	5.12408(6)	14.1289(3)	0.011(2)	0.976(4)	0.35709(7)	0.1485(3)	0.3181(2)	0.0227(2)	0.24575(7)	0.0210(4)	0.0221(4)	2.90
600	5.11265(5)	14.0993(3)	0.007(1)	0.984(2)	0.35663(6)	0.1483(2)	0.3178(2)	0.0226(2)	0.24568(6)	0.0172(3)	0.0187(3)	2.92

ilm100

20	5.08795(4)	14.0880(2)	0.013(1)	0.974(2)	0.35572(4)	0.1465(1)	0.3181(1)	0.0242(1)	0.24518(3)	0.0060(1)	0.0081(2)	3.06
200	5.09997(5)	14.1147(2)	0.009(1)	0.982(2)	0.35613(5)	0.1468(1)	0.3186(2)	0.0247(1)	0.24512(4)	0.0102(2)	0.0117(2)	3.14
400	5.10937(5)	14.1403(2)	0.008(2)	0.984(4)	0.35654(5)	0.1470(1)	0.3190(2)	0.0251(1)	0.24517(4)	0.0131(2)	0.0143(2)	2.95
500	5.11441(5)	14.1537(3)	0.009(2)	0.982(4)	0.35675(5)	0.1470(1)	0.3192(2)	0.0250(1)	0.24509(5)	0.0140(2)	0.0154(2)	2.89
600	5.11988(5)	14.1668(3)	0.012(2)	0.976(4)	0.35691(5)	0.1473(1)	0.3196(2)	0.0251(1)	0.24509(5)	0.0148(2)	0.0162(2)	2.79
700	5.12579(5)	14.1797(3)	0.012(2)	0.976(4)	0.35709(6)	0.1474(1)	0.3198(2)	0.0250(2)	0.24504(5)	0.0158(3)	0.0172(3)	2.78
800	5.13157(5)	14.1967(3)	0.012(2)	0.976(4)	0.35734(6)	0.1473(1)	0.3202(2)	0.0252(2)	0.24508(5)	0.0176(3)	0.0184(3)	2.77
900	5.13730(5)	14.2165(3)	0.014(2)	0.972(4)	0.35749(7)	0.1476(2)	0.3209(2)	0.0256(2)	0.24520(6)	0.0202(3)	0.0209(3)	2.73
1000	5.14373(6)	14.2358(3)	0.018(2)	0.964(4)	0.35786(8)	0.1474(2)	0.3212(3)	0.0260(2)	0.24525(7)	0.0244(4)	0.0241(4)	2.82
1100	5.15116(7)	14.2522(4)	0.025(2)	0.950(4)	0.35827(10)	0.1472(2)	0.3211(3)	0.0262(2)	0.24547(8)	0.0301(6)	0.0290(5)	2.96
1200	5.16015(8)	14.2653(4)	0.050(2)	0.900(4)	0.35871(12)	0.1474(3)	0.3208(4)	0.0259(3)	0.24582(10)	0.0352(9)	0.0334(8)	2.96
1250	5.16622(9)	14.2697(5)	0.070(3)	0.860(6)	0.35892(13)	0.1474(4)	0.3200(4)	0.0250(3)	0.24628(12)	0.0339(4)	0.0326(4)	2.95

Table 2

1300	5.17269(9)	14.2678(5)	0.103(3)	0.794(6)	0.35934(15)	0.1476(5)	0.3202(4)	0.0239(3)	0.24659(13)	0.0356(5)	0.0334(4)	2.87
1325	5.17665(9)	14.2653(5)	0.134(3)	0.732(6)	0.35956(18)	0.1475(7)	0.3188(4)	0.0222(4)	0.24705(15)	0.0340(6)	0.0316(4)	2.85
1200	5.16334(10)	14.2742(6)	0.063(3)	0.874(6)	0.35876(15)	0.1470(4)	0.3198(5)	0.0257(3)	0.24651(14)	0.0269(5)	0.0277(5)	3.61
1000	5.14823(6)	14.2478(3)	0.019(2)	0.962(4)	0.35787(8)	0.1474(2)	0.3214(3)	0.0260(2)	0.24520(7)	0.0243(3)	0.0244(3)	2.83
800	5.13586(6)	14.2139(3)	0.016(2)	0.968(4)	0.35736(7)	0.1471(2)	0.3206(3)	0.0255(2)	0.24526(6)	0.0163(2)	0.0175(2)	2.97
600	5.12481(5)	14.1826(27)	0.013(2)	0.974(4)	0.35688(6)	0.1469(1)	0.3201(2)	0.0252(2)	0.24519(5)	0.0143(2)	0.0157(2)	3.05