

Chemistry of black leaf films synthesised with rail steels and its influence on low friction mechanism

Kei Ishizaka ^{a, b}, Stephen R Lewis ^{a, c}, Deborah Hammond ^d and Roger Lewis ^{*a}

^a Department of Mechanical Engineering, The University of Sheffield, Mappin Street, Sheffield S1 3JD, UK

^b East Japan Railway Company, 2-2-2 Yoyogi, Shibuya-ku, Tokyo 151-0053, Japan

^c British Steel, Scunthorpe Rail and Section Mill, Brigg Road, Scunthorpe, DN16 1BP

^d Sheffield Surface Analysis Centre, Department of Chemistry, The University of Sheffield, Dainton Building, Brook Hill, Sheffield S3 7HF

Supplementary Information

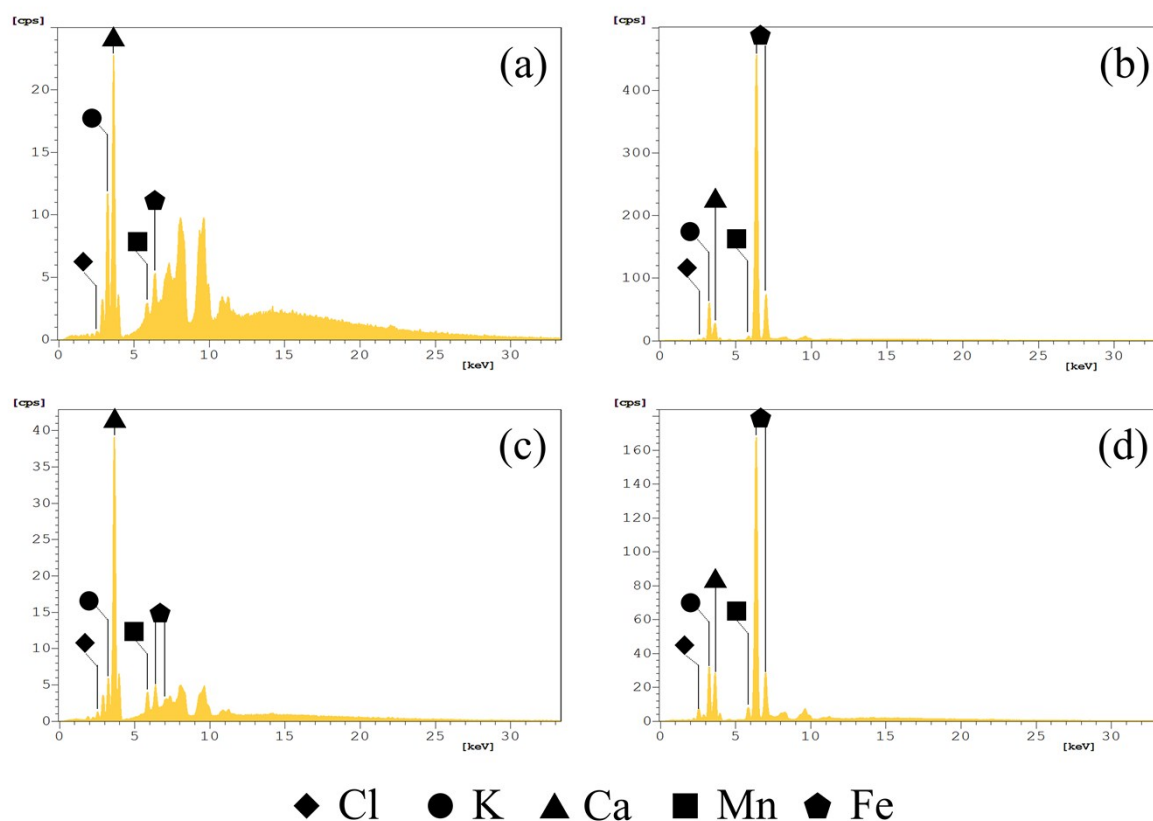
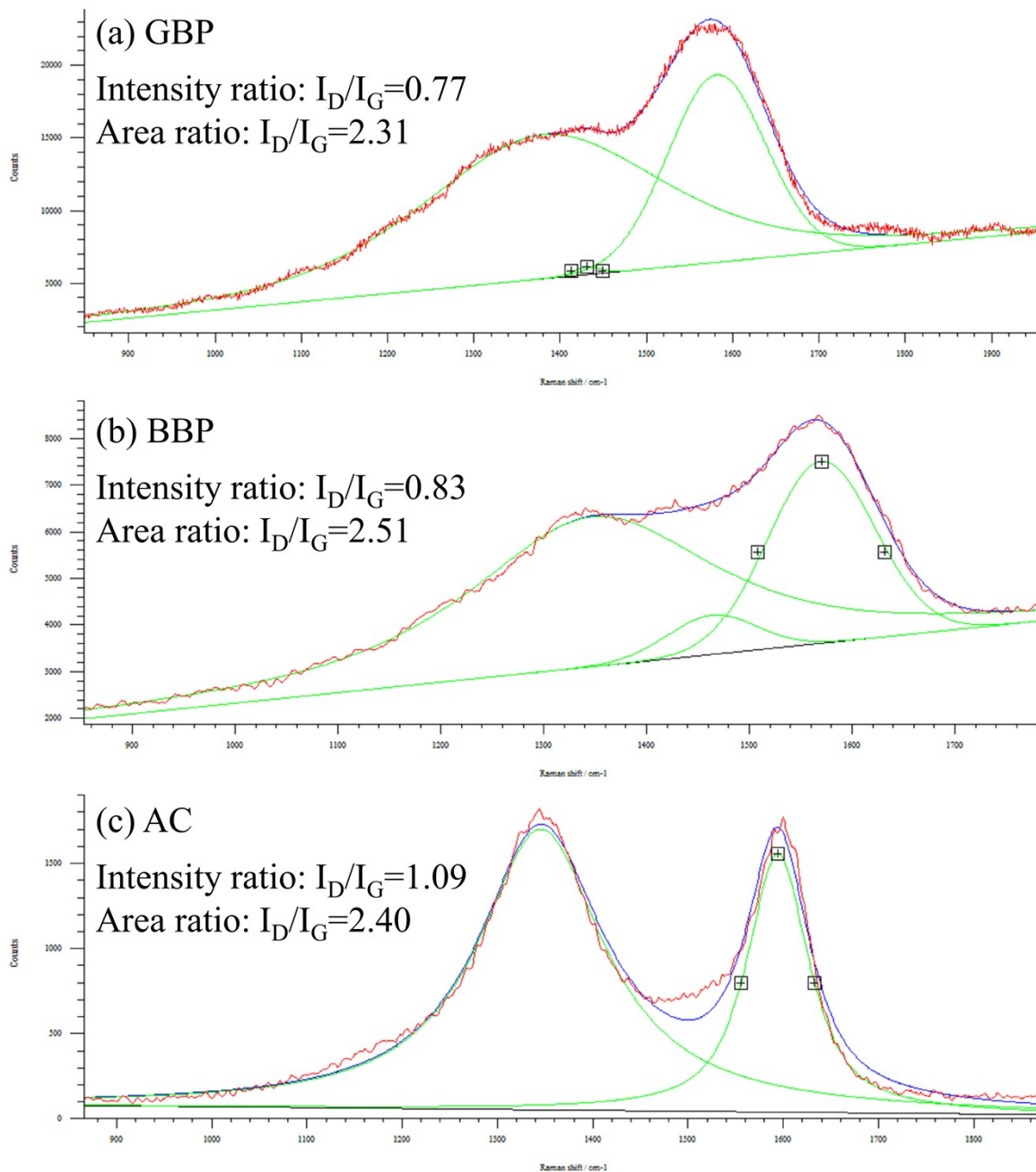


Figure S1 XRF results: (a) GLP, (b) GBP, (c) BLP, (d) BBP

Table S1 Assignments of XRD peaks measured in BBP

Measured 2θ	2θ in reference	Assignment
14.7	14.6208	CaSO ₄
20.7	-	-
25.51	25.4645	CaSO ₄
28.31	28.3453	KCl
29.09	29.1521	CaSO ₄
29.51	29.4867	CaSO ₄
31.05	-	-
31.69	31.8395	CaSO ₄
40.48	40.5074	KCl
49.02	49.0628	CaSO ₄
50.15	50.1688	KCl
53.8	53.8096	CaSO ₄
58.58	58.6402	KCl
66.35	66.3809	KCl
73.67	73.7331	KCl

KCl: PDF number 00-041-1476
CaSO₄: PDF number 04-016-3271



**Figure S2 peak fittings of the acquired Raman spectra
 (a) GBP, (b) BBP, (c) Activated charcoal**

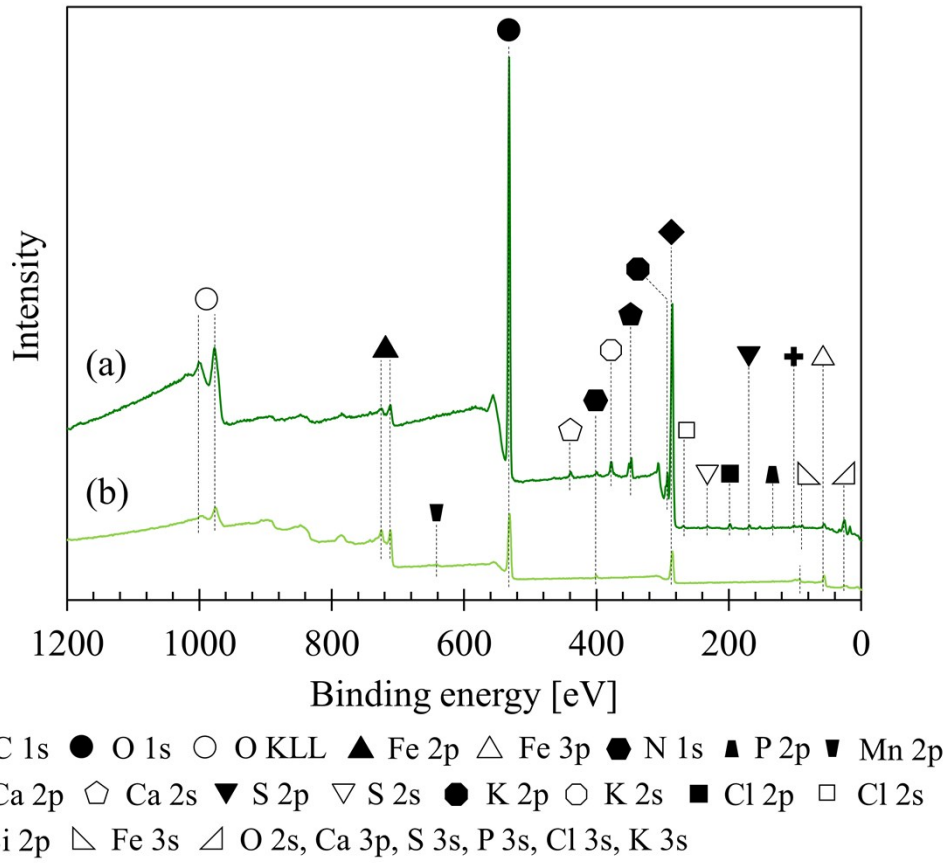
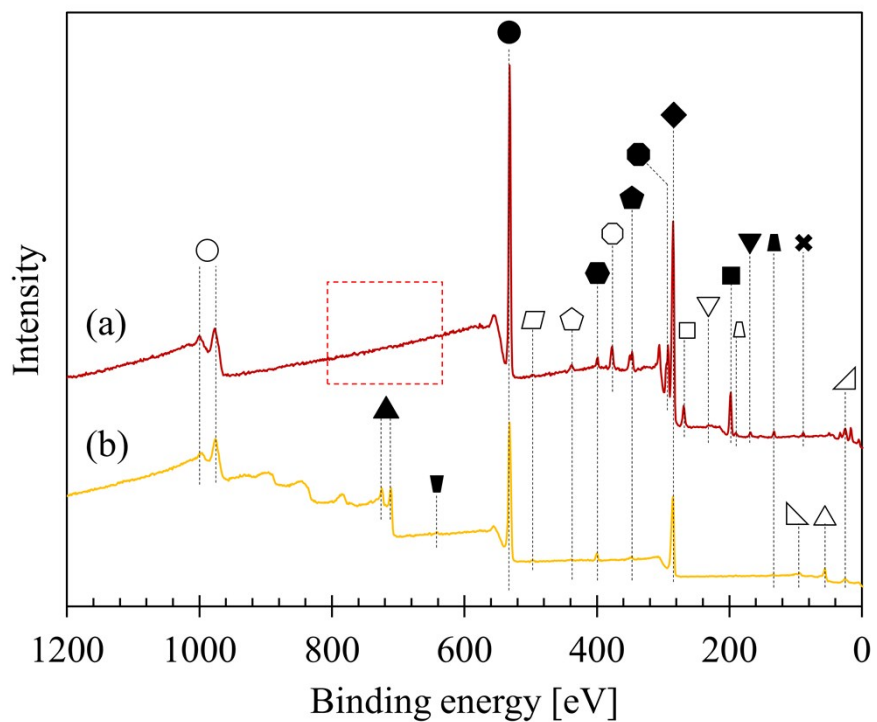


Figure S3 XPS results of GBP: (a) Thick GBP film, (b) Thin GBP film



- ◆ C 1s ● O 1s ○ O KLL ▲ Fe 2p △ Fe 3p ● N 1s ▲ P 2p △ P 2s
 ✖ Mg 2s ▼ Mn 2p ● Ca 2p ◊ Ca 2s ▼ S 2p ▽ S 2s ● K 2p ○ K 2s
 ■ Cl 2p □ Cl 2s ◊ Na KLL △ Fe 3s △ O 2s, Ca 3p, S 3s, P 3s, Cl 3s, K 3s

Figure S4 XPS results of BBP: (a) Thick BBP film, (b) Thin BBP film

Table S2 Main findings in the material analyses

Analysis	Main findings
XRF	<ul style="list-style-type: none">• Fe ions are dissolved into LEs and cause the chemical reaction• Graphitic carbon covers the surface of BP
RS	<ul style="list-style-type: none">• This structure is often seen in RS spectra of a sugar-derived carbon• Iron oxides are underneath the carbon surface
XPS	<ul style="list-style-type: none">• BP mainly consists of carbon, oxygen, iron and nitrogen• Oxidised graphite might exist according to the chemical shifts of C 1s and O 1s• The thick organic layer is formed on the surface of BBP, covering iron oxides• The relatively high concentration of phosphate is detected only in heated BBP
FT-IR	<ul style="list-style-type: none">• Chelate structure of iron-carboxylate seems to be formed