Colloidal origin of microbands in banded iron formations

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Supplementary Information

The Supplementary Information includes:

- Geological Overview
- Methods
- Table S-1
- XRD Patterns
- Figures S-1 to S-5
- Supplementary Information References

Geological Overview

Figure S-1  Overview of the geology and stratigraphy of the Hamersley Province, Western Australia (modified after Taylor et al., 2001). Study area: Turner Syncline (box); Ages (t) are based on Trendall et al. (2004); metamorphic zones are identified as Z1: prehnite-pumpellyite facies, high zeolite facies; Z2: prehnite-pumpellyite facies; Z3: pumpellyite-actinolite facies; Z4: greenschist zone (Smith et al., 1982).
**Methods**

The samples were analysed by scanning electron microscopy (SEM) using a JEOL 7001F FEG-SEM with an energy dispersive X-ray spectrometer (EDS) operating at an accelerating voltage of 15 kV and a probe current of 1.1 nA. Quantitative powder X-ray diffraction (XRD) data were reduced by Rietveld refinement (Rietveld, 1969; Hill et al., 1987; Bish and Howard, 1988); XRD patterns were collected using a PANalytical MPD diffractometer with a Co X-ray tube operated at 40 kV and 40 mA. Data for mineral identification and Rietveld refinement were collected over a range of 5–140° 2θ using an X'Celerator linear position sensitive detector. Refinements were done using the program Topas v.4.2 from Bruker AXS and the fundamental parameters approach (Cheary and Coelho, 1992).

**Supplementary Table**

Table S-1 XRD data of selected samples.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Quartz (%)</th>
<th>Hematite (%)</th>
<th>Goethite (%)</th>
<th>Kaolinite (%)</th>
<th>Total</th>
<th>Rwp</th>
<th>d (nm)</th>
<th>(\chi^2)</th>
<th>CS_L (nm)</th>
<th>Lvol-IB (nm)</th>
<th>Lvol-FWHM (nm)</th>
<th>S_L (nm)</th>
<th>Description</th>
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</thead>
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<tr>
<td>A-1</td>
<td>85.4</td>
<td>14.1</td>
<td></td>
<td>0.5</td>
<td>100.0</td>
<td>7.7</td>
<td>0.8</td>
<td>2.2</td>
<td>164</td>
<td>105</td>
<td>146</td>
<td>0.039</td>
<td>Chert with intragranular particles</td>
</tr>
<tr>
<td>B-1</td>
<td>88.3</td>
<td>11.5</td>
<td>0.2</td>
<td></td>
<td>100.0</td>
<td>7.6</td>
<td>0.8</td>
<td>2.2</td>
<td>113</td>
<td>72</td>
<td>101</td>
<td>0.063</td>
<td>Chert with intragranular particles</td>
</tr>
<tr>
<td>C-1</td>
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<td>10.0</td>
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<td>7.7</td>
<td>1.0</td>
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<td>114</td>
<td>0.200</td>
<td>Chert with intragranular particles</td>
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<tr>
<td>C-2</td>
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<td>10.2</td>
<td></td>
<td></td>
<td>100.0</td>
<td>9.3</td>
<td>1.1</td>
<td>2.6</td>
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<td>68</td>
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<td>0.134</td>
<td>Chert with intragranular particles</td>
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<td>0.3</td>
<td>3.5</td>
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<td>107</td>
<td>150</td>
<td>0.036</td>
<td>Quartz with intergranular hematite/microbands</td>
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<td>49.8</td>
<td>0.5</td>
<td></td>
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<td>2.1</td>
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<td>108</td>
<td>151</td>
<td>0.129</td>
<td>Quartz with intergranular hematite/microbands</td>
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<td>2.0</td>
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<td>106</td>
<td>149</td>
<td>0.123</td>
<td>Quartz with intergranular hematite/microbands</td>
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Sample co-ordinates

<table>
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<tr>
<th>Sample</th>
<th>Co-ordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>22°45’2.96” S, 117°32’39.12” E</td>
</tr>
<tr>
<td>B</td>
<td>22°44’27.31” S, 117°44’26.66” E</td>
</tr>
<tr>
<td>C</td>
<td>22°45’46.66” S, 117°45’20.12” E</td>
</tr>
</tbody>
</table>

**Abbreviations**

- **Rwp**: Weighted pattern index, a function of the least-squares residual
- **d**: Durbin-Watson statistics, a measure of serial correlation for the least-squares fit
- **\(\chi^2\)**: Reduced chi-squared statistic for the least-squares fit
- **CS_L**: Crystallite size using a Lorentzian convolution
- **Lvol-IB**: Volume weighted column height, dimensional length
- **Lvol-FWHM**: Scherrer’s equation with full weighted column height of the pure Lorentzian function
- **S_L**: Microstrain; modeled using a Lorentzian convolution
XRD Patterns
B-1

Quartz low: 87.99%
Hematite: 11.86%
Goethite: 0.15%

B-1

Quartz low: 87.99%
Hematite: 11.86%
Goethite: 0.15%
B-3

- Quartz low: 49.02%
- Hematite: 50.61%
- Goethite: 0.37%

B-3

- Quartz low: 49.02%
- Hematite: 50.61%
- Goethite: 0.37%
Supplementary Figures

Figure S-2  Photomicrograph inset (XPL) of Figure 1a. Strong differences in crystallographic preferred orientations (CPO) of quartz are highlighted by gypsum plate analysis (Egglseeder et al., 2016). Layers rich in colloidal hematite (red, brown) lack CPOs, whereas interlayered hematite and quartz layers (bottom) as well as quartz-dominated layers (top) show strong CPOs.

Figure S-3  TEM images and selected area electron diffraction (SAED) patterns of hematite from iron-oxide bands in the Kuruman Iron Formation, South Africa (Sun et al., 2015: Figs. 6A, 6B): Although, Sun et al. (2015) identify that hematite nanoparticles are comprised of “nano-domains” of 3-5 nm in size, which represent individual crystals, we suggest that these nanocrystals form by dehydration of ferrihydrite and coarsening to larger nanoparticles by Ostwald ripening. The interface misorientations of adjacent nanocrystals are features formed by oriented attachment, instead of crystallisation by dissolution-precipitation. From Sun et al., 2015, with permission from Geological Society of America.
Figure S-4  TEM image of hematite from the Kuruman Iron Formation, South Africa (Sun et al., 2015: Fig. 8B). The lattice fringes of adjacent hematite nanocrystals show interface misorientations, which is evidence for particle-based crystallisation instead of dissolution-precipitation. From Sun et al., 2015, with permission from Geological Society of America.

Figure S-5  TEM image of hematite from lateritic soils from Brazil (Orberger et al., 2014; Fig. 11 H). Interface misorientations of adjacent hematite nanocrystals are interpreted as "twinning" and compared to BIF from India. However, we suggest instead that these misorientations of lattice fringes are related to imperfect oriented attachment of hematite nanoparticles. From Orberger et al., 2014, with permission from Springer Nature.
Supplementary Information References


