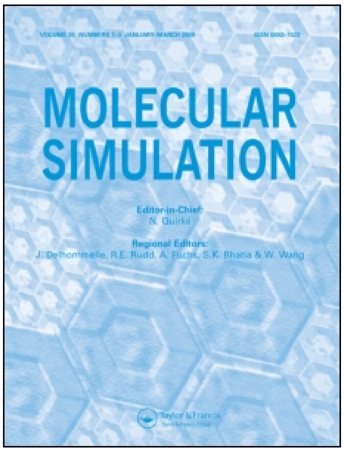

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Minerals Processing in South Africa: Materials Modelling Opportunities

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MINERALS PROCESSING IN SOUTH AFRICA: MATERIALS MODELLING OPPORTUNITIES

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Opportunities for materials modelling in the minerals industry are reviewed, with the South African minerals industry as an example. This industry is the main contributor to export earnings for the country, and research and development in this field is essential, owing to the decline in mineral-processing research developed countries.

The main processes for the recovery of gold, platinum-group metals, ferrous metals, non-ferrous metals, and industrial minerals are described technically, and the opportunities for modelling are discussed, with the emphasis on industrial applications.

Materials modelling has an important role to play in the development of more efficient and selective reagents, more valuable materials, new uses for primary commodities, and in the examination of systems that defy experimentation. Closer collaboration between academic institutions and commercial R & D organizations should be initiated to persuade the latter of the value of materials modelling.

Keywords: Minerals processing; materials modelling applications

INTRODUCTION

In the past two decades, profound changes have taken place in the mineral industry worldwide. In the developed world, the industry has declined significantly for several reasons, the most important being the perception that it is a significant contributor to pollution, and the fact that mineral resources in these countries have been largely depleted. Research in mineral science in these countries has also declined in proportion, and several well-known research laboratories, such as the US Bureau of Mines, and Warren Spring Laboratories in the UK have closed down. Production of mineral commodities has shifted to the developing countries, but their capacity for maintaining the same levels of R & D as the developed countries, is severely limited. Countries such as Australia, Brazil, Chile, and South Africa will have to rely on their own research resources to develop new processes and to optimize existing ones. Materials modelling, with the focus on applied research, can become a cost-effective alternative to expensive experimentation. This paper discusses some opportunities, particularly for modelling systems that are difficult to investigate experimentally.

SOUTH AFRICA'S MINERALS INDUSTRY

The minerals industry in South Africa is a very important one, with total sales in 1996 amounting to US $13 000 million. In spite of the fact that it contributes only 8.1 per cent to the Gross Domestic Product of the country, the minerals industry's contribution to total exports is 41 per cent. It is therefore the most important generator of export revenue, and this will remain so in the foreseeable future. The country is also blessed with an abundance of mineral resources, and it has the most important resource base in many commodities [1], as can be seen in Figure 1.

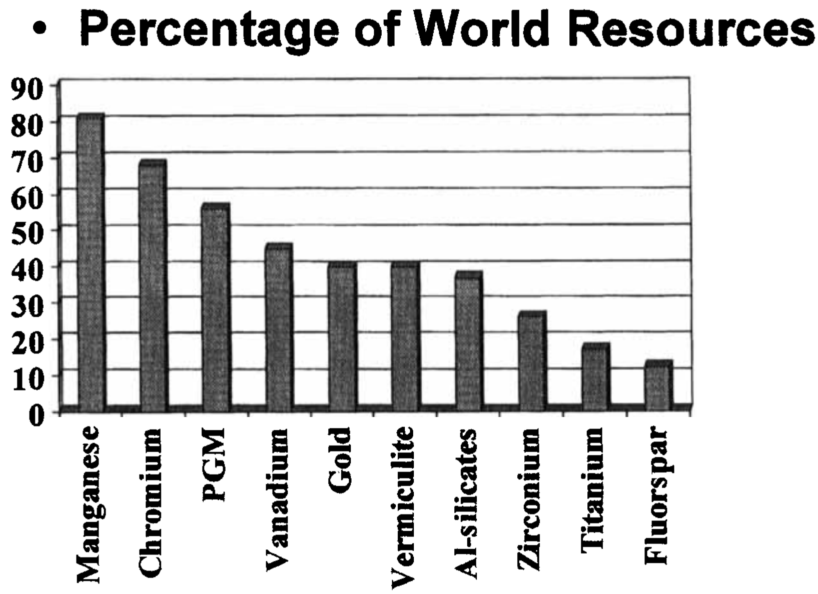

FIGURE 1 South Africa's proportion of world mineral resources.

The industry is, however, under threat because of a decline in commodity prices in real terms over the past two decades [2]. It is therefore focussing on efficiency in the extraction and production of these commodities. Research and development is therefore essential for its profitability and eventual survival.

THE GOLD INDUSTRY

Metallurgical Processes

The gold industry has evolved over the past century into a highly efficient one, which can extract gold from ores with concentrations of 1 gram per tonne or less. Several processes exist, with the carbon-in-pulp process as the most recently developed. A schematic representation of the process is shown in Figure 2.

The gold ore is milled and treated with a cyanide solution to dissolve the gold. The solution is contacted with activated carbon in a countercurrent fashion, in which the most highly loaded carbon is in contact with the most concentrated solution, and the least loaded, regenerated carbon is in contact with the most dilute gold solution. The loaded carbon is then stripped with a concentrated cyanide solution, and the gold electrolytically precipitated,

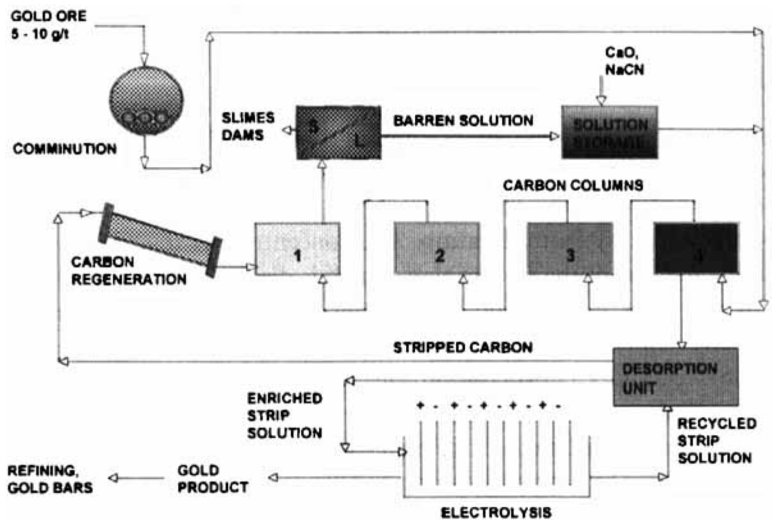

FIGURE 2 Metallurgical processes – gold.

and smelted into gold bars after further refinement. Recent developments involve the use of ion-exchange resin instead of carbon for increased gold extraction and higher selectivity, especially in the presence of metals such as copper and zinc, which compete with the gold when loading on the activated carbon.

Materials Modelling Opportunities

In gold processing, the following aspects could be of relevance:

- The development of selective resins for the recovery of copper, cyanide, and gold from copper-gold ores, which are particularly troublesome to process. These metals and reagents must be selectively isolated and recovered.
- The modelling of so-called molecular recognition compounds for specific elements could lead to novel reagents that, if grafted onto resins, will give increased selectivity for the absorption of gold and other elements from solution.
- The development of new alloying elements for the replacement of allergenic nickel in jewellery, and of hard, durable 24-carat jewellery, which is popular in Asian countries.

THE PLATINUM GROUP METALS INDUSTRY

Metallurgical Processes

The two major producers of platinum-group metals (PGMs) are South Africa and the Russian Republic, with lesser production from the USA, Canada, and Zimbabwe. The process (Fig. 3) is based on milling followed by concentration by froth flotation. The concentrate is smelted to separate the sulfide melt from the silicate slag, which is discarded. The sulfide melt is then treated in a Peirce–Smith converter to remove the iron and some sulfur. The copper–nickel sulfide product is then leached to produce copper, nickel, and a PGM concentrate, which is further refined to produce the pure metals.

The presence of deleterious elements such as chromium, selenium, and tellurium give rise to problems during smelting and refining, and interaction between the slag and furnace refractories can lead to catastrophic failures in equipment.

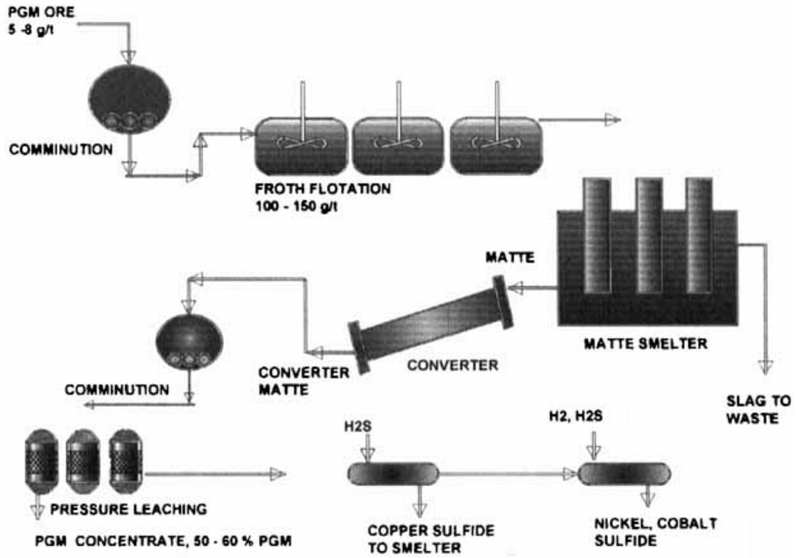

FIGURE 3 Metallurgical processes – platinum group metals.

Materials Modelling Opportunities

In spite of decades of development and optimization of the flotation process, average recoveries still remain around 80 per cent. Opportunities exist to model the effect of flotation reagents and depressants on sulfide flotation, which is still poorly understood for minerals containing platinum-group elements.

With the development of new refining processes based on ion exchange, there is a need to further optimize the efficacy of molecular recognition compounds for increased selectivity. The development of novel catalysts based on platinum-group elements could be facilitated by the use of materials modelling. Particularly the use of elements such as ruthenium, iridium and osmium could be investigated.

New coloured platinum alloys for jewellery applications have been developed, mainly by trial and error. Through modelling, the most desirable candidates could be identified and developed.

Modelling could facilitate the development of new corrosion-resistant alloys and electrode coatings containing platinum group elements.

THE FERROUS METALS INDUSTRY

Metallurgical Processes

The ferrous metals industry is an exciting and challenging one in South Africa. In addition to various grades of stainless steel, ferro-alloys such as ferrochromium, ferromanganese, silicomanganese, ferrovanadium, ferrosilicon, and ferrotitanium are produced. Normally, the ores are smelted with appropriate reductants in large electric-arc furnaces to produce various grades of these alloys (Fig. 4). In the case of ferrochromium, the hot alloy is decarburized in argon-oxygen or vacuum decarburization furnaces to produce alloy for the production of stainless steel.

The main problems associated with ferro-alloy production are related to the extent of reduction of the ores. The quality of stainless steel and the presence of inclusions are important issues requiring research.

Materials Modelling Opportunities

Several models have been proposed to elucidate the reduction mechanisms and reduction kinetics in oxide minerals. These range from gaseous

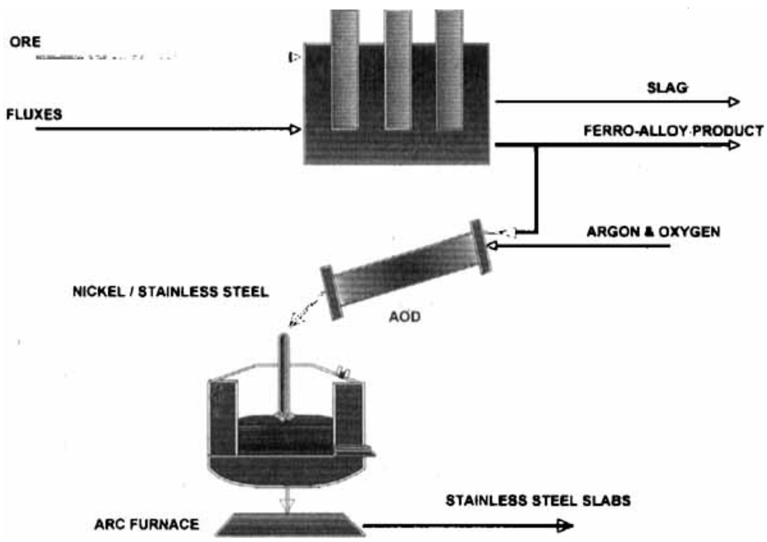

FIGURE 4 Metallurgical processes – ferro-alloys.

reduction to reduction in the solid state, where vacancy migration plays an important part. Modelling of these reduction mechanisms could assist in optimizing the reduction behaviour of chromium and manganese ores. Low-nickel stainless steel alloys have been under development to replace nickel-bearing grades, since nickel constitutes the largest proportion of the raw materials cost. Modelling could assist in developing the most appropriate alloys, and also in the development of corrosion resistant alloys.

NON-FERROUS METALS

Metallurgical Processes

These processes are diverse, and very different for the various metals such as aluminium, magnesium, copper, nickel, and titanium. Here the focus will be on the base metals industry. Figure 5 shows one of the processes for the production of copper from sulfide ores.

The ore is milled and concentrated using froth flotation. After roasting to remove some of the sulfur, the concentrate is smelted and the sulfide melt is further treated in a converter to remove iron and sulfur. The impure metal is cast into anodes and purified using electrolysis.

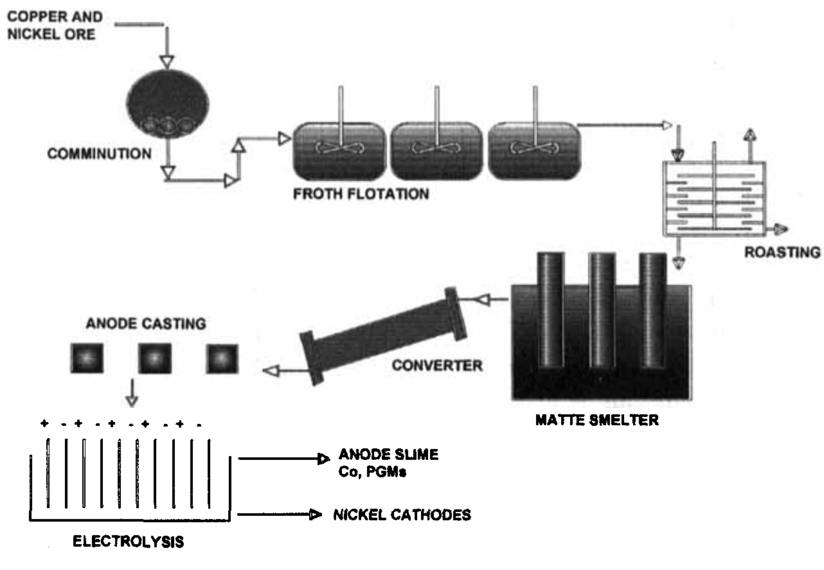

FIGURE 5 Metallurgical processes – copper/nickel.

Materials Modelling Opportunities

The flotation response of the various minerals containing copper and other base metals have been investigated for many years, and the opportunities for modelling the interaction between the minerals and the various flotation reagents could provide new impetus to develop more effective reagents.

The leaching properties of the various minerals, particularly the copper minerals, also offer promise for materials modelling. Bacterially assisted leaching of the more refractory minerals such as chalcopyrite remains a challenge, and the modelling of passivation effects could lead to a better understanding of leaching mechanisms.

Materials modelling could facilitate the development of selective solvent-extraction and ion-exchange reagents for the separation of nickel and cobalt.

The modelling of metal-to-carbide bonding mechanisms for the manufacture of more durable drill bits and cutting tools is also a possibility.

INDUSTRIAL MINERALS

Metallurgical Processes

Because of the diverse nature of the metallurgical processes for the production of industrial minerals, an example of only one such process is given – the production of titanium metal and titanium dioxide pigment, which is shown schematically in Figure 6.

Titanium minerals are usually derived from beach sands by gravity, electrostatic, and magnetic separation to produce rutile (TiO_2) and ilmenite ($FeTiO_3$) concentrates. The rutile can be used directly as chlorination feedstock. The ilmenite is smelted in electric-arc furnaces to produce a high grade titania slag and high quality pig iron. The slag is then also used as chlorination feedstock. The titanium tetrachloride from carbo-chlorination is then purified and used for the production of titanium metal *via* the Kroll process, which uses magnesium metal as a reductant. Alternatively, titanium dioxide pigments can be produced by oxidation of the $TiCl_4$.

Materials Modelling Opportunities

Several opportunities exist for materials modelling. The ilmentite concentrate is usually treated in a roasting step to increase its magnetic susceptibility. This step is necessary to separate impurities, such as chromite,

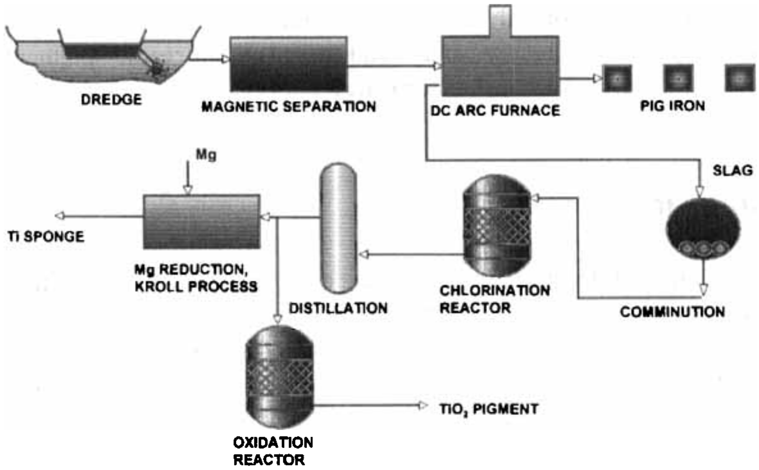

FIGURE 6 Metallurgical processes – titanium.

from ilmenite. Modelling will increase our knowledge of the factors that could influence roasting and magnetic separation.

The modelling of the conductivity of rutile is another interesting possibility with practical applications. Rutile is usually separated from other non-magnetic phases by electrostatic separation. Its conductivity (also its electrostatic properties) can be modified by heat treatment under varying redox conditions, or by treating the material with surfactants. Modelling can point to the most appropriate treatment options.

The calculation of the thermodynamic properties of various phases probably offers the most exciting practical application of materials modelling. In the case of titanium processing, the thermodynamic properties of the TiO_2 polymorphs are well known. These phases have been extensively modelled, and transferable interatomic potentials have been derived. Comparison of the calculated and experimentally derived thermodynamic properties of these compounds should provide a good test for the capabilities of this approach. Calculated thermodynamic properties of other titanium oxide phases such as the Magneli phases would also be useful, since they are almost impossible to synthesize in pure form.

Other areas involving the modelling of industrial minerals could be the following:

- Modification of the functionality and compatibility of inorganic fillers and stabilizers in polymers such as polyvinyl chloride.
- Surface modification of catalyst support materials

- Modelling of photocatalytic effects in oxide materials, notably TiO_2.
- Modification of opacity and brightness of inorganic pigments by application of various surface coatings.

CONCLUSIONS

Research and development in developing countries, including South Africa, are increasingly focussing on applied research because of limited financial and manpower resources. Materials modelling can provide a cost-effective alternative to expensive and protracted experimental investigations. It is also applicable to materials and processes that are difficult to investigate experimentally.

Probably the most promising application of materials modelling is the calculation of thermodynamic properties of materials using crystallographic structure data and transferable interatomic potentials. This could provide valuable data for a large number of compounds, for which no data exist at present.

Close collaboration between academic and commercial research and development organizations is recommended to provide proper focus on the systems to be investigated and modelled. The value of materials modelling will become apparent when some of these systems are comprehensively modelled.

References

[1] Chamber of Mines of South Africa (1996). "South African Mining Industry Statistical Tables".
[2] Crowson, P. (1996). "Minerals Handbook 1996–97", MacMillan Press Ltd.