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Reducing polysilicon materials costs

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ABSTRACT
It is well known that the cost of silicon materials is the major cost factor in crystalline silicon PV module production. Polysilicon price accounts for about 30% of total module production costs. While the PV industry has set a polysilicon price target of US$40/kg by 2015, this goal will not be reached if demand continues to exceed supply and if new plants cannot reduce operating costs below US$25/kg. Given a continued 30% annual growth in demand for PV modules, new polysilicon plants and expansions are needed to avoid shortages of high-purity, cost-effective polysilicon. This paper discusses the major factors in polysilicon production costs, the important elements of polysilicon plant design for reducing operating costs, the key cost elements of polysilicon plant operations, and how the design of polysilicon products can reduce crystal growth costs.

Polysilicon demand and supply

Government solar energy associations around the world have detailed their national policies on solar energy at recent conferences. A summary of the national plans charts a continued annual growth rate of over 30% through the next ten years [1,2,3]. Crystalline silicon PV module demand is projected to continue at an average annual growth rate of 30% for the same period, resulting in a demand of over 1 million metric tons of polysilicon per year by 2020. Since worldwide polysilicon production was about 130,000 tons in 2010, production volume will have to increase by 800% to meet demand in 2020. However, polysilicon supply has been increasing at a rate of only 20–22% per year. Even with significant gram/watt conversion rate improvements, polysilicon demand will exceed projected supply, creating shortages that will result in high prices if a number of new plants are not built over the next three years. To avoid a shortage, several new plants and expansions are required, designed for producing high-purity polysilicon at an operating cost < US$25/kg.

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Cost element	Cost/kg of polysilicon (US$)
Trichlorosilane production	9–12
Electricity	3.5–7
Labour	3.5–5
Materials	2
Maintenance	2
Amortization	0–10
Total	20–38

Table 1. Polysilicon production costs for the Western nation polysilicon suppliers.

Polysilicon production cost elements

The estimated polysilicon production costs for the Western nation polysilicon suppliers are shown in Table 1.

Trichlorosilane production costs

Trichlorosilane (TCS, $SiHCl_3$), used to produce polysilicon, is synthesized either by *direct chlorination*, the exothermic reaction of metallurgical-grade silicon (MG Si) and hydrogen chloride (HCl), or by *hydrochlorination*, the endothermic reaction of MG Si and silicon tetrachloride (STC, $SiCl_4$) in a hydrogen atmosphere. Production costs of TCS range from US$1.50 to $2.00/kg depending on production volume, MG Si cost, HCl or STC cost, TCS yield, electrical power rates, labour and utility costs.

After synthesis, the TCS is purified in a series of distillation columns designed to produce 11-nines (99.999999999 weight %) purity polysilicon with a minimal loss of chlorosilanes. The losses of chlorosilanes in the production and purification process have a major impact on operating costs and can be held to less than 15%. The weight of silicon in the trichlorosilane molecule is 20.6%, so the maximum conversion of TCS to polysilicon is 4.9:1. The 1–2% impurities in MG Si are reduced to sub-part-per-billion (sub-ppb) trace levels by converting to chlorosilane, chloride and hydride compounds, which accounts for the losses in trichlorosilane.

With a purification system based on impurity thermodynamic data, computer simulation and operational plant experience, the ratio of TCS to polysilicon is 6:1. This assumes recovery of the co-product gases, especially the STC. If the STC is not recovered from the synthesis reaction and from the chemical vapour deposition (CVD) reactor vent gas, the ratio of TCS to polysilicon is 20:1. TCS production costs range from about US$1.50 to $2.00/kg, so the conversion ratio determines the cost element of TCS

TCS production costs	@$1.50/kg	@$1.75/kg	@$2.00/kg
	($/kg)	($/kg)	($/kg)
Conversion ratio TCS:poly 6:1	9.00	10.50	12.00
Conversion ratio TCS:poly 8:1	12.00	14.00	16.00
Conversion ratio TCS:poly 10:1	15.00	17.50	20.00
Conversion ratio TCS:poly 20:1	30.00	35.00	40.00

Table 2. Effect of the conversion ratio of TCS to polysilicon on polysilicon production costs.

in the final polysilicon product as shown in Table 2. Poorly designed distillation systems with an excessive number of columns, high chlorosilane losses and/or poor STC recovery systems have a significant impact on operating costs. These systems must be upgraded to realize major cost reductions.

Item	USA	MENA	Korea	China	Europe
Electricity ($/kWh)	0.03–0.04	0.035	0.055	0.04–0.07	0.11
Labour ($/yr/person)	75,000	70,000	60,000	20,000	75,000
Water ($/ton)	0.26	1.60	0.26	0.26–0.5	2.2
Support	good	good	good	limited	limited

Table 3. Comparison of regional sites for polysilicon plants.

Electricity, utility and labour costs

Electricity rates are region and site specific and subject to unexpected increases. This is a major factor in site selection and it is the primary reason that new plants and expansions are limited in Europe. In addition to low rates, the electrical power must be non-interruptible, meet technical specifications and be available in long-term contracts. Two separate feed lines coming into the plant minimize the risk of power failure, which is a critical safety issue in a polysilicon plant; moreover, unplanned outages can cost tens of millions dollars in lost production. Per kg of polysilicon, total electrical power consumption for an entire plant ranges from about 90 to over 140kWh. Electrical use is reduced by use of steam, recovery of process heat, use of energy-efficient equipment and overall plant design for energy efficiency. Power consumption for TCS production, purification, deposition, and gases recovery is shown in Table 4.

Utilities are also site specific and vary greatly from region to region. The availability of hydrogen and nitrogen gases, fresh water and natural gas must also be considered in site selection. In some remote areas, hydrogen and nitrogen, in addition to HCl, must be synthesized. This adds to the operating costs as well as to capital expenditure (capex). Labour rates are similar from country to country, except for the much lower rates currently available in China.

Government support for polysilicon plants varies greatly from country to country and also within a country. Support may include tax incentives, government-backed loans, free or inexpensive land, and building of roads, as well as job training and other support services. While these can reduce capex, the effect on the 10-year amortization portion of polysilicon production costs is small compared to the lower costs of electrical and utilities over an operating life of 30+ years. A comparison of regional sites is charted in Table 3.

Amortization cost

Today's polysilicon plants are often being built at 10,000 MTY (metric tons/year) capacities to achieve economy of scale and reduce labour cost per kg. Capex ranges from US$800 million to $1.1 billion depending on whether the site is 1) an expansion of an existing facility with roads, rail, land, buildings and all utilities available; 2) a brownfield site/industrial park, with roads, utilities and access established; or 3) a greenfield site, where transportation access, land and utilities must be installed. For a 10-year amortization period, US$8–$11/kg is added to operational costs, not including interest on the capital expense. With this large burden on production costs, the remaining cost elements must be reduced below US$25/kg to yield a return on investment and to allow for investment in future expansion. The PV industry polysilicon price target of US$40/kg requires an energy-efficient, high-productivity plant design on a site with favourable power, labour and utilities costs.

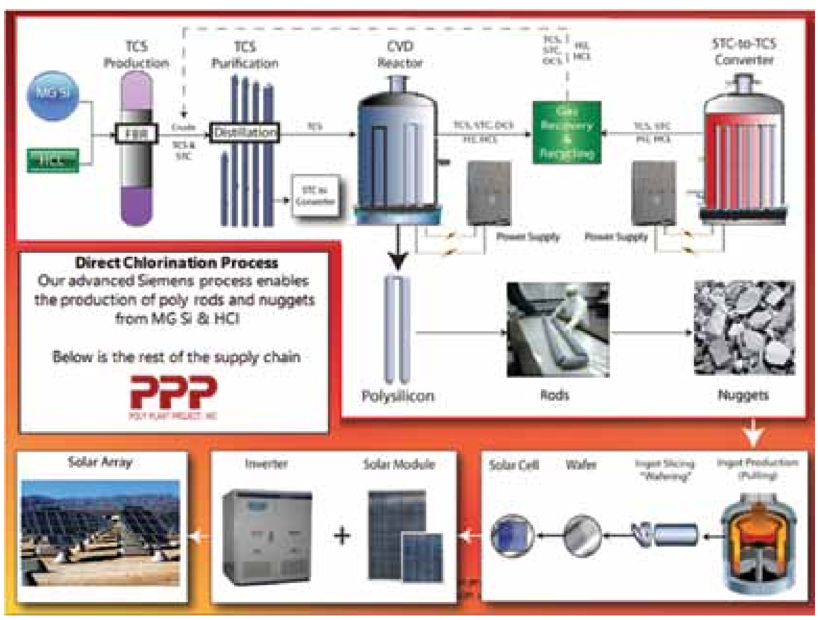

Figure 1. Representation of the direct chlorination process for producing trichlorosilane.

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Polysilicon plant design

The key elements of polysilicon plant design are listed below.

Trichlorosilane synthesis technology

TCS is synthesized by hydrochlorination or by direct chlorination. The hydrochlorination reaction, also called *hydrogenation*, is written as: MG Si + $2H_2$ + $3SiCl_4$ = $4HSiCl_3$; original work on this process was described in an early patent [4] and developed in production volumes by Union Carbide in 1984 [5]. Four polysilicon suppliers now use this process to produce TCS-based polysilicon. The direct chlorination reaction, also called the *Siemens process*, is written as: MG Si + 3HCl = $SiHCl_3$ + H_2 and has been in use since the early 1950s. Most polysilicon suppliers use this process for TCS-based polysilicon.

In the hydrochlorination process, co-product gases are recycled in the synthesis fluid bed reactor, using co-product STC as the chlorine source, which eliminates the need for HCl and for STC-to-TCS thermal converters; therefore, the operating cost for the hydrochlorination process is about 10% lower than the operating cost for the direct chlorination process on the same site. A comparison of the two technologies is shown in Table 4.

Item	Hydrochlorination	Direct chlorination
MG Si use (kg/kg poly)	1.05	1.26
HCl use (kg/kg poly)	0	0.74
STC use (kg/kg poly)	0.25	0
Hydrogen use (kg/kg poly)	0.11	0.1
Reaction temperature (°C)	~550	~350
Reaction pressure (bar g)	~30	~5
TCS yield (mol %)	26 to 30	> 90
Electrical energy (kWh/kg poly)	65	75
STC converter (mol % yield)	not required	22%
Capex (normalized)	1.0	1.05

Note: both processes produce STC as a co-product. In the hydrogenation process, the STC is recycled in the TCS synthesis reactor; in the direct chlorination process, the STC is recycled in a separate thermal conversion reactor.

Table 4. Comparison of hydrochlorination and direct chlorination TCS synthesis technologies.

Trichlorosilane purification

An advanced TCS purification system is a combination of distillation and adsorption columns that uses computer simulation with data from operating systems to design the number of trays, reflux ratios, column sizes and number of columns to efficiently purify the TCS with less than 15% losses of chlorosilanes and a 6:1 TCS to polysilicon ratio. An efficient design must take into consideration over 50 different chemical species, with thermodynamic and binary interaction parameters defined for each species.

Energy conservation

To reduce the electrical power costs, energy conservation measures must be implemented throughout the entire plant design. Two major conservation areas are heat recovery from the process equipment and energy-efficient equipment design. The largest energy savings, about 50%, have been realized in the advanced CVD reactor designs with larger capacity, as shown in Table 5.

Co-product gases recovery and recycling

As discussed above, the co-product STC must be recycled to achieve economical use of TCS. Hydrogen and HCl are also recovered and recycled. The materials consumption in Table 4 assumes recovery and recycling of gases.

Plant size

Prior to 1999, 2500 MTY was considered to be a large-capacity plant, since demand was from the semiconductor industry with only a 10% annual growth rate. With the large PV market averaging a 30% growth rate, polysilicon plants are designed for 10,000 MTY to meet growing demand and achieve economy of scale. The larger plants have reduced labour costs and are able to negotiate for lower utility rates and quantity discounts for materials. A limitation on capacity is the ability to contract for sufficient electrical power, water, materials and utilities.

Polysilicon specifications

The plant design must include design of the distillation system for the required polysilicon purity and design of the product handling facility to meet the product specifications. Defining a purity specification for solar-grade polysilicon (SOG) has been problematic, with values ranging from 6 to 11 nines. This is calculated as silicon weight % based on acceptor and donor impurities only. Since a crystalline silicon ingot of 0.1Ωcm *p*-type has a boron dopant level of 2ppmw, the starting polysilicon feedstock must have a purity of at least 7 nines to minimize impurity interferences from the feedstock. SOG polysilicon at 8 or 9 nines, based on acceptor and donor content, is recommended to avoid feedstock resistivity contamination in crystal growth.

The higher purity levels may require additional equipment in the distillation system and/or higher reflux ratios, so capital expense and operating costs may be higher. Electronic-grade (EG) purity is usually specified at sub-ppb levels for donor and acceptor with smooth polysilicon rod surface texture. The smooth surface requires slower growth rates in the CVD reactor, resulting in higher power consumption. An automated rod-breaking system, clean-room processing, surface etching of chunk polysilicon product, and packaging in 5kg clean bags are also required. In addition to increased capital expense, operating costs are higher and can increase by as much as US$8 to $12/kg for EG polysilicon [6].

	rods	kWh/kg	tons/yr
Small	12–24	90–200	80–150
Standard	36	60–70	180–260
Advanced	48–54	< 50	375–500

Table 5. Comparison of energy use for larger capacity CVD reactors.

Redundancy

Redundancy in process design and for key equipment must be included in the polysilicon plant design. It is imperative to avoid long downtimes: a month-long shutdown for a 10,000 MTY plant can result in a US$50 million loss in sales income. A loss this large can justify redundancy in design and operation. Long shutdowns can be avoided by installing two independent electrical feed lines to the plant, installing sufficient TCS storage, building adequate stores of materials and equipment spare parts, preparing for fast maintenance response and adopting safe and reliable operating practices.

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Safe operation

Safety must be an integral part of the plant design since hazardous gases at high temperatures and pressures, high voltage power supplies, crane operations, high structures and heavy loads are some of the risks. A comprehensive, thorough safety system – including facilities and equipment, training and information, policies and procedures, and emergency preparedness – is required to mitigate the risks. The consequences of injury to the workforce or of damage to property or the environment can be far-reaching and lead to long shutdowns, plant closures or liability actions.

Polysilicon plant operations

Even with an efficient plant design and advanced equipment, high productivity is necessary to meet the goal of < US$25/kg production costs. Key elements in achieving high productivity are as follows.

24/7 plant operation

The plant must be fully staffed in order to provide continuous operation throughout the year. Periodic shutdowns for maintenance or equipment installations must be planned so that CVD reactor operations can continue. This requires adequate TCS storage and redundancy in TCS production.

Operator training

With operational experience, processes become more efficient and bottlenecks are identified and corrected.

Process engineering

The implementation of industrial engineering principles, especially product flow and logistics through the polysilicon processing area, results in a large gain in productivity. For a 10,000 MTY plant using CVD reactors at 400 tons/yr capacity and an 84-hour run cycle, a reactor must be started every 3.5 hours.

Quality control

Quality-control procedures for each process step, from incoming materials to the final product, are required in order to maximize yields and to prevent product loss. A comprehensive laboratory is used to evaluate incoming materials, examine TCS purity and analyze product purity. Daily lab data is used for process control in the TCS, polysilicon deposition and polysilicon product areas.

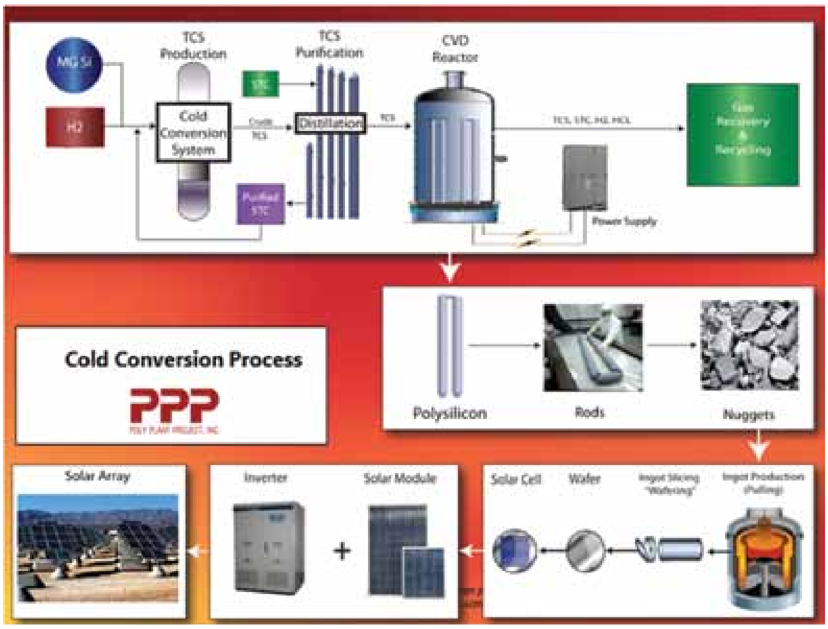

Figure 2. Representation of the hydrochlorination process (cold conversion) for producing trichlorosilane.

Design of polysilicon products

Designing polysilicon specifications for the various crystal growth methods can reduce crystal growth costs. Close cooperation between the polysilicon supplier and the ingot grower can significantly reduce ingot growth costs. Cooperative studies have demonstrated cost reductions in the following areas.

Purity specification

Metals concentration in silicon wafers is known to degrade solar cell minority-carrier lifetime values and resultant cell efficiency. The primary source of metals contamination in TCS-based polysilicon is the contamination of the surface during product processing and packaging. For EG polysilicon, surface metals are specified at less than 10ppbw [7], requiring a surface chemical etch and expensive product handling and packaging. Defining a specification limit for SOG at higher levels, based on ingot and cell lifetime measurements, allows less expensive product processing and bulk packaging.

Bulk packaging

Typical packaging for EG polysilicon is

Figure 3. CVD reactors in the polysilicon plant deposition building.

5kg polyethylene bags in a 30kg carton. Six cartons are required for a Czochralski (Cz) crucible load of 180kg, and 17 cartons for a directional solidification system (DSS) crucible load of 510kg. For SOG poly, 140kg cartons or 1 ton bulk packaging can be used. Package materials and storage costs and packaging and unpacking labour costs result in savings of up to US$1/kg.

Polysilicon form and size

Maximum packing of the crucible, with the optimal mixture of rod sections, chunks and chips, increases crystal ingot weight per run and improves productivity, which reduces ingot growth costs. Granular and chip-form polysilicon have a bulk density of about 1.5g/cc, chunks about 1.7g/cc and rod sections about 2g/cc. The use of an optimal mix can increase ingot weight by 10%.

Load and melt time

Rod sections can be loaded faster than chunks and chips, saving polysilicon load time. In addition, rod sections and large chunks have better bulk thermal conductivity than chips and granules, which reduces the melt time in the crystal growth furnace.

Continuous feed and recharge of crucibles

For Cz growth furnaces, the open crucible allows better packing density and the opportunity to continuously feed or recharge polysilicon. Some vendors provide continuous feed capability for the Cz growth furnace by using granular or chip-form polysilicon to provide a continuous feed into the crucible. A technical concern has been the presence of dislocations and crystal faults caused by introducing cold, solid polysilicon into the hot melt, disturbing melt thermal stability. While these are not acceptable for semiconductor-grade ingots, some level of dislocations is acceptable for solar-grade ingots. Recharge systems are another approach to achieving continuous growth. After the initial ingot growth, the remaining melt is recharged with granules or polysilicon rods, then a second ingot is grown. The major cost benefit of a recharge system is the extension of crucible life to three to five pulls, thereby reducing crucible cost; other cost benefits are an increase in energy efficiency and in hot zone life.

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Conclusions

PV module installations are expected to continue at annual growth rates of 30% for the next several years, with crystalline silicon as the dominant technology. Because polysilicon production is increasing at only 20–22% per year, many new plants will need to be built to avoid shortages. These plants must be designed for cost-efficient production of high-purity material, and the polysilicon product must be designed to reduce ingot growth costs and improve electrical characteristics. The major cost factors in polysilicon production have been reviewed, along with key elements of plant design and operations. To effectively reduce total silicon materials costs, the polysilicon supplier must establish cooperative technical programmes with the ingot supplier to define optimal polysilicon specifications, from purity to packaging.

With demand increasing faster than supply, and taking into account the high amortization costs for existing plants, it is unlikely that polysilicon prices will meet the US$40/kg PV industry target over the next ten years, but will remain in the current US$50–$55/kg contract price range. Vertical integration offers several advantages to the PV module supplier, beyond assurance of supply. A cost-effective polysilicon plant would supply production volumes at a US$25 to $30/kg transfer price; provide polysilicon products designed to reduce ingot costs; and design products to meet advanced solar cell requirements.

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About the Author

Jan Maurits has over 40 years’ experience in the silicon industry, including 16 years’ at a major polysilicon supplier, with experience in polysilicon products development, Q.A., analytical methods development, technical marketing and product management. He has published 22 technical papers and made numerous presentations at technical conferences. Jan is co-founder and President of Poly Plant Project, Inc., a specialty engineering company formed in 2005 to provide consulting services, process technology and key equipment for production of high-purity, cost-effective polysilicon.

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